LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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: VX042376.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	22	28	42	rBV2	23935	39370	15.69%	1.527%
2	1.374	43	47	48	rBV4	5049	6117	2.44%	0.237%
3	2.270	189	194	203	rBV	29542	50929	20.30%	1.975%
4	2.721	262	268	273	rBV	14075	30850	12.30%	1.196%
5	3.063	318	324	332	rVB2	1544	3339	1.33%	0.129%
6	3.416	376	382	387	rBV5	918	1955	0.78%	0.076%
7	3.593	405	411	421	rBV5	1173	3674	1.46%	0.142%
8	3.849	446	453	463	rVV2	1755	5276	2.10%	0.205%
9	4.276	515	523	532	rVB5	2395	6270	2.50%	0.243%
10	4.501	552	560	581	rBV	11068	44995	17.93%	1.745%
11	5.056	640	651	666	rBV	26413	81614	32.53%	3.165%
12	5.263	682	685	687	rBV2	116	178	0.07%	0.007%
13	5.446	700	715	727	rBV7	4081	14225	5.67%	0.552%
14	5.550	727	732	733	rBV3	672	917	0.37%	0.036%
15	5.812	769	775	776	rBV3	1201	1844	0.73%	0.072%
16	5.958	790	799	817	rBV3	75331	214691	85.57%	8.326%
17	6.111	822	824	825	rVV2	622	549	0.22%	0.021%
18	6.135	825	828	837	rVV3	929	2217	0.88%	0.086%
19	6.239	840	845	851	rVB2	658	1492	0.59%	0.058%
20	6.342	856	862	869	rBV5	1666	4003	1.60%	0.155%
21	6.598	899	904	910	rBV5	1013	2052	0.82%	0.080%
22	6.757	922	930	946	rBV	87708	211282	84.21%	8.194%
23	7.111	987	988	996	rVB2	390	514	0.20%	0.020%
24	7.226	1002	1007	1013	rBV4	475	893	0.36%	0.035%
25	7.306	1013	1020	1026	rBV2	41101	93669	37.33%	3.633%
26	7.489	1045	1050	1053	rBV2	305	423	0.17%	0.016%
27	7.586	1063	1066	1069	rVV2	120	198	0.08%	0.008%
28	7.653	1071	1077	1082	rVB2	1060	1896	0.76%	0.074%
29	7.763	1088	1095	1102	rVB5	1184	2573	1.03%	0.100%
30	7.891	1114	1116	1121	rBV2	126	161	0.06%	0.006%
31	7.952	1121	1126	1133	rVV4	1250	2424	0.97%	0.094%
32	8.177	1156	1163	1166	rBV4	545	970	0.39%	0.038%
33	8.220	1168	1170	1174	rVB2	376	398	0.16%	0.015%
34	8.275	1174	1179	1182	rBV3	1480	2448	0.98%	0.095%
35	8.324	1182	1187	1195	rBV	20847	36014	14.35%	1.397%
36	8.427	1201	1204	1212	rVB4	870	1536	0.61%	0.060%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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	8.598	1226	1232	1234	rBV2	3907	6423	2.56%	0.249%
38	8.647	1234	1240	1248	rVV	101501	165622	66.01%	6.423%
39	8.720	1248	1252	1257	rVB	12795	18392	7.33%	0.713%
40	8.842	1265	1272	1279	rVB4	1272	2888	1.15%	0.112%
41	8.909	1279	1283	1286	rBV3	2895	4017	1.60%	0.156%
42	8.958	1286	1291	1302	rVV2	15254	30775	12.27%	1.194%
43	9.049	1304	1306	1308	rVV	230	208	0.08%	0.008%
44	9.098	1308	1314	1320	rVB3	1356	2128	0.85%	0.083%
45	9.226	1333	1335	1337	rBV3	202	161	0.06%	0.006%
46	9.275	1339	1343	1349	rVB3	1438	2343	0.93%	0.091%
47	9.336	1349	1353	1354	rBV	146	210	0.08%	0.008%
48	9.397	1356	1363	1375	rBV	43087	102374	40.80%	3.970%
49	9.616	1395	1399	1403	rBV3	3790	5245	2.09%	0.203%
50	9.750	1416	1421	1426	rBV3	693	1375	0.55%	0.053%
51	9.817	1427	1432	1442	rVB3	3463	6079	2.42%	0.236%
52	9.903	1442	1446	1453	rBV4	1416	2287	0.91%	0.089%
53	10.006	1458	1463	1465	rBV2	993	1320	0.53%	0.051%
54	10.055	1465	1471	1481	rBV	173936	242792	96.77%	9.416%
55	10.201	1490	1495	1500	rVB	4795	6927	2.76%	0.269%
56	10.299	1502	1511	1517	rBV	17164	30198	12.04%	1.171%
57	10.451	1533	1536	1539	rVB2	576	643	0.26%	0.025%
58	10.592	1551	1559	1563	rBV4	1990	4366	1.74%	0.169%
59	10.640	1563	1567	1577	rVB	16712	24021	9.57%	0.932%
60	10.750	1581	1585	1586	rBV3	1826	1924	0.77%	0.075%
61	10.781	1587	1590	1594	rVB2	4184	5327	2.12%	0.207%
62	10.854	1599	1602	1605	rVV3	3863	5520	2.20%	0.214%
63	10.890	1605	1608	1612	rVB	4353	6234	2.48%	0.242%
64	10.964	1615	1620	1624	rBV	4963	6509	2.59%	0.252%
65	11.031	1628	1631	1635	rBV5	1308	1792	0.71%	0.069%
66	11.195	1652	1658	1670	rVB	89825	122624	48.87%	4.756%
67	11.305	1672	1676	1680	rBV2	3576	5531	2.20%	0.215%
68	11.384	1685	1689	1694	rVV	5045	7769	3.10%	0.301%
69	11.433	1694	1697	1702	rVV4	4924	10858	4.33%	0.421%
70	11.476	1702	1704	1714	rVB2	8936	12706	5.06%	0.493%
71	11.573	1718	1720	1722	rBV2	288	259	0.10%	0.010%
72	11.616	1723	1727	1733	rBV	3428	5446	2.17%	0.211%
73	11.713	1740	1743	1744	rBV3	4971	5683	2.27%	0.220%
74	11.860	1763	1767	1769	rBV4	3635	4845	1.93%	0.188%
75	11.939	1776	1780	1783	rBV5	3937	6180	2.46%	0.240%
76	12.024	1789	1794	1800	rBV	195061	250898	100.00%	9.731%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

77	12.091	1801	1805	1811	rVB2	5302	9379	3.74%	0.364%
78	12.323	1837	1843	1850	rBV	136784	181602	72.38%	7.043%
79	12.421	1856	1859	1864	rBV	9780	10993	4.38%	0.426%
80	12.530	1874	1877	1879	rBV4	1634	2052	0.82%	0.080%
81	12.683	1899	1902	1904	rBV3	1226	1475	0.59%	0.057%
82	12.762	1913	1915	1918	rBV3	916	916	0.37%	0.036%
83	12.860	1928	1931	1934	rBV5	3682	5474	2.18%	0.212%
84	12.975	1946	1950	1955	rVB5	3307	4464	1.78%	0.173%
85	13.268	1994	1998	2008	rVB3	9177	14722	5.87%	0.571%
86	13.384	2014	2017	2019	rBV3	4425	5761	2.30%	0.223%
87	13.579	2046	2049	2051	rBV3	1552	1880	0.75%	0.073%
88	13.780	2077	2082	2088	rVB	26531	37527	14.96%	1.455%
89	13.841	2088	2092	2096	rBV2	7684	9294	3.70%	0.360%
90	14.036	2121	2124	2129	rBV2	7469	8545	3.41%	0.331%
91	14.426	2184	2188	2196	rBV2	11740	18184	7.25%	0.705%
92	14.640	2215	2223	2228	rBV	23774	38139	15.20%	1.479%
93	14.780	2239	2246	2253	rVB2	25639	40237	16.04%	1.561%
94	14.932	2269	2271	2276	rVB4	5966	6163	2.46%	0.239%
95	15.414	2346	2350	2356	rVB4	29644	43130	17.19%	1.673%
96	15.481	2357	2361	2367	rVV4	8284	14660	5.84%	0.569%
97	15.615	2378	2383	2386	rBV	12672	20621	8.22%	0.800%
98	15.737	2395	2403	2411	rVB7	13030	31822	12.68%	1.234%
99	15.987	2440	2444	2447	rBV3	20230	32420	12.92%	1.257%
100	16.024	2447	2450	2457	rVB2	28105	46129	18.39%	1.789%

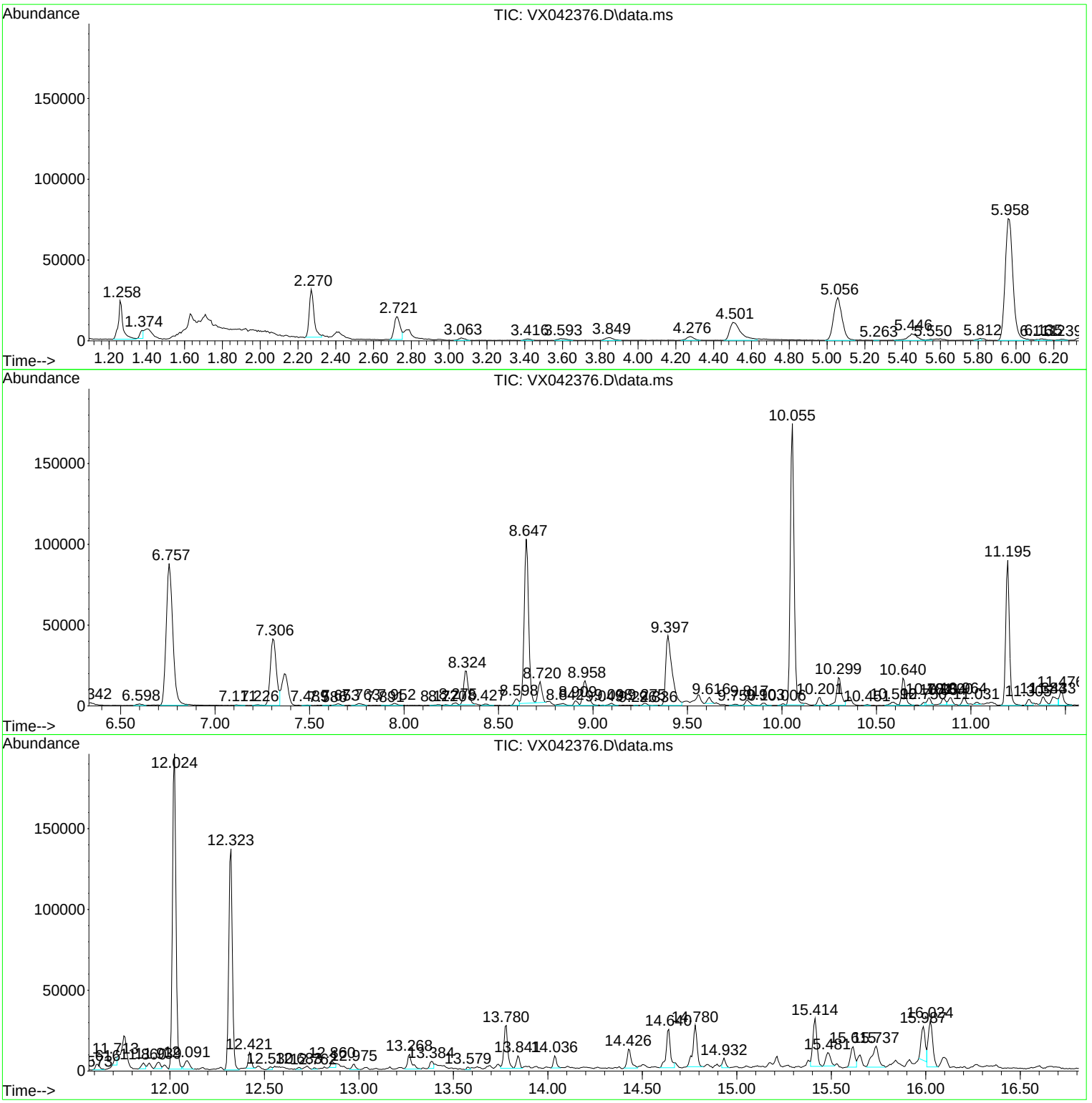
Sum of corrected areas: 2578444

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

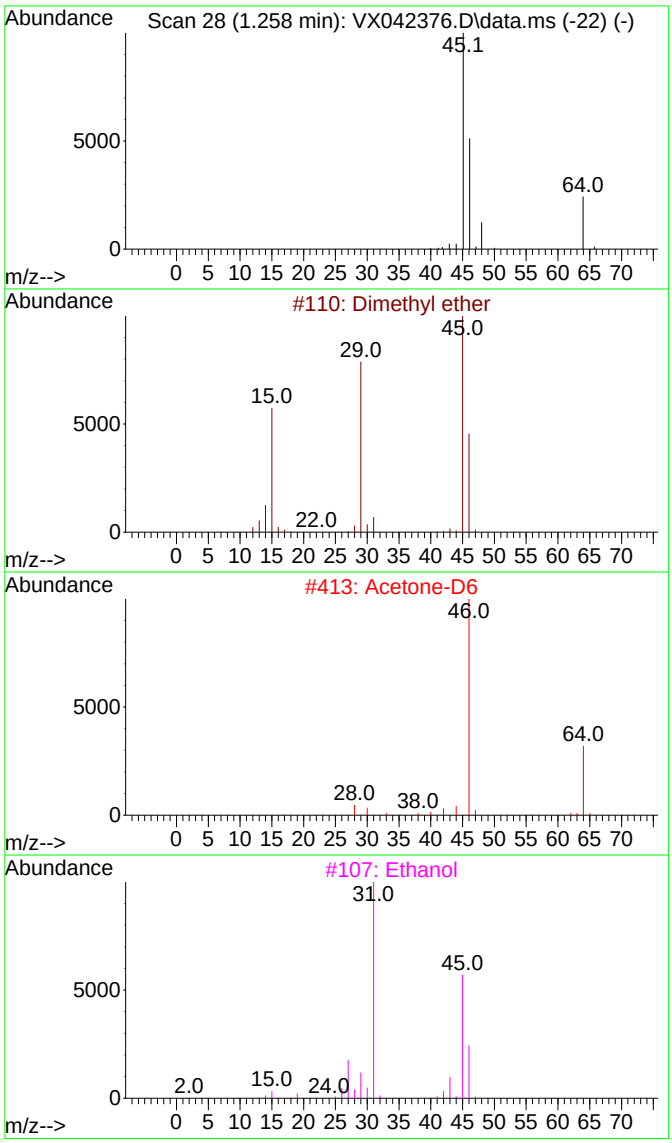
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

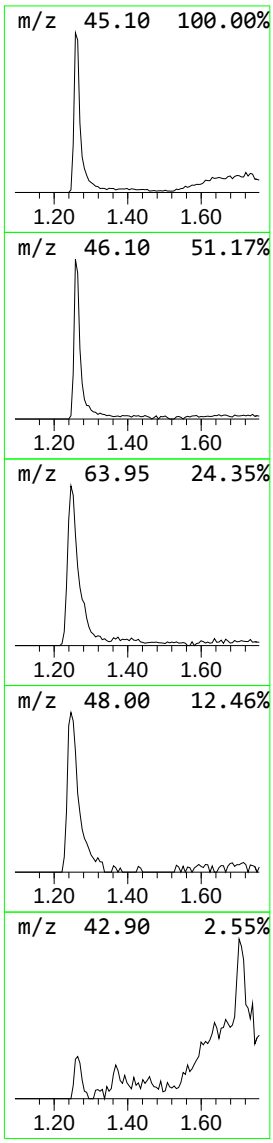
****

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	9.32 ug/L	39370	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	45
2	Acetone-D6	64	C3D6O	000666-52-4	30
3	Ethanol	46	C2H6O	000064-17-5	9
4	Acetone-D6	64	C3D6O	000666-52-4	9
5	Dimethyl ether	46	C2H6O	000115-10-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

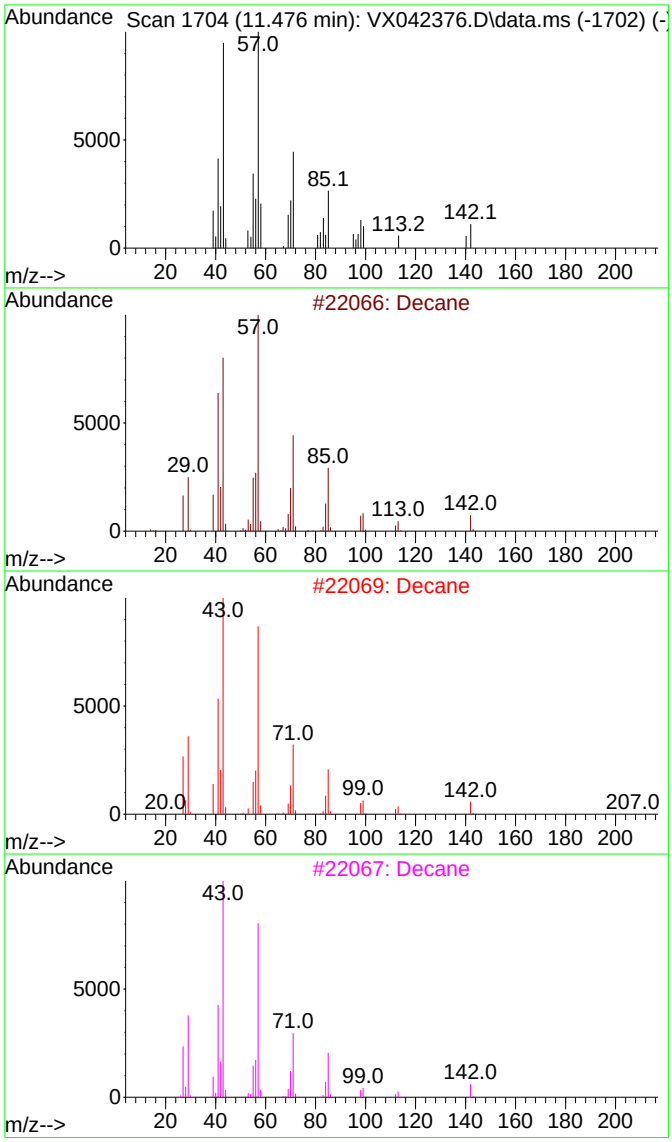
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

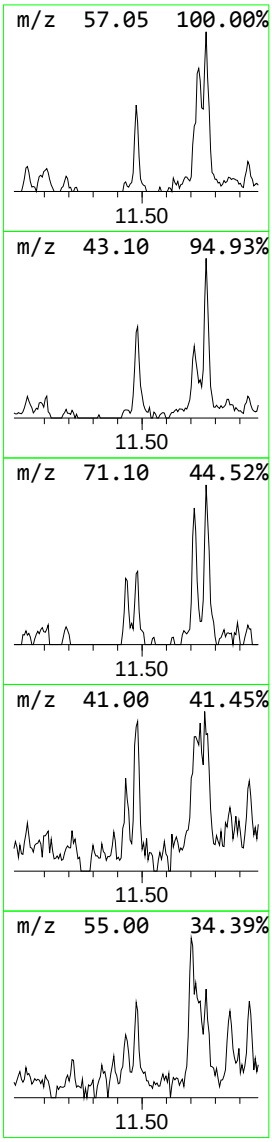
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.476	2.53 ug/L	12706	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane	142	C10H22	000124-18-5	93
2	Decane	142	C10H22	000124-18-5	81
3	Decane	142	C10H22	000124-18-5	72
4	Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	52
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

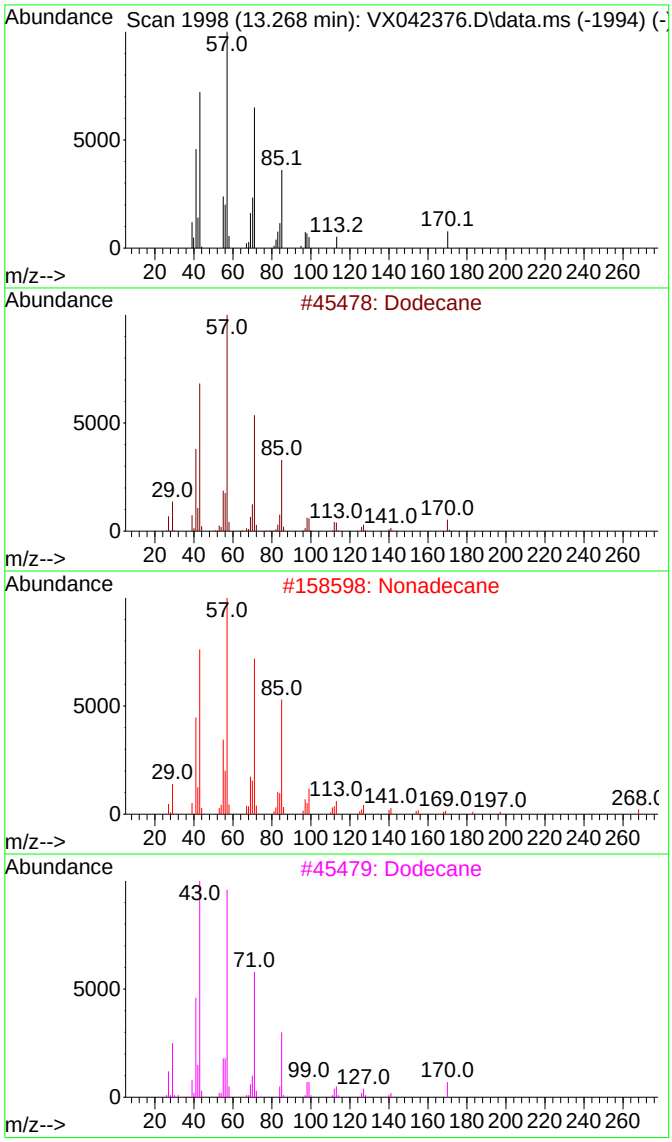
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

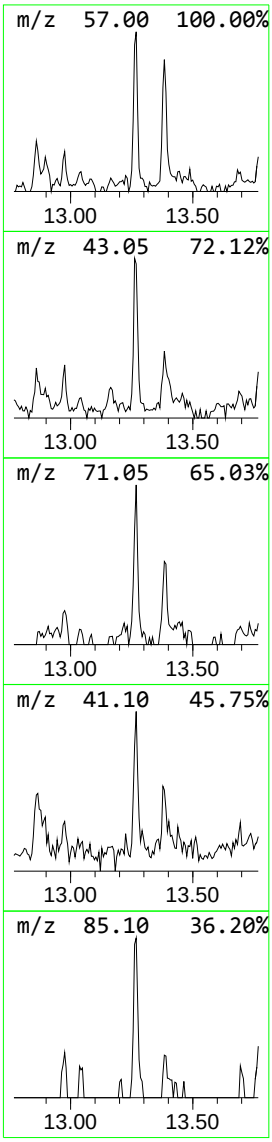
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	2.93 ug/L	14722	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	87
2	Nonadecane	268	C19H40	000629-92-5	80
3	Dodecane	170	C12H26	000112-40-3	80
4	Hexadecane	226	C16H34	000544-76-3	72
5	Dodecane	170	C12H26	000112-40-3	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

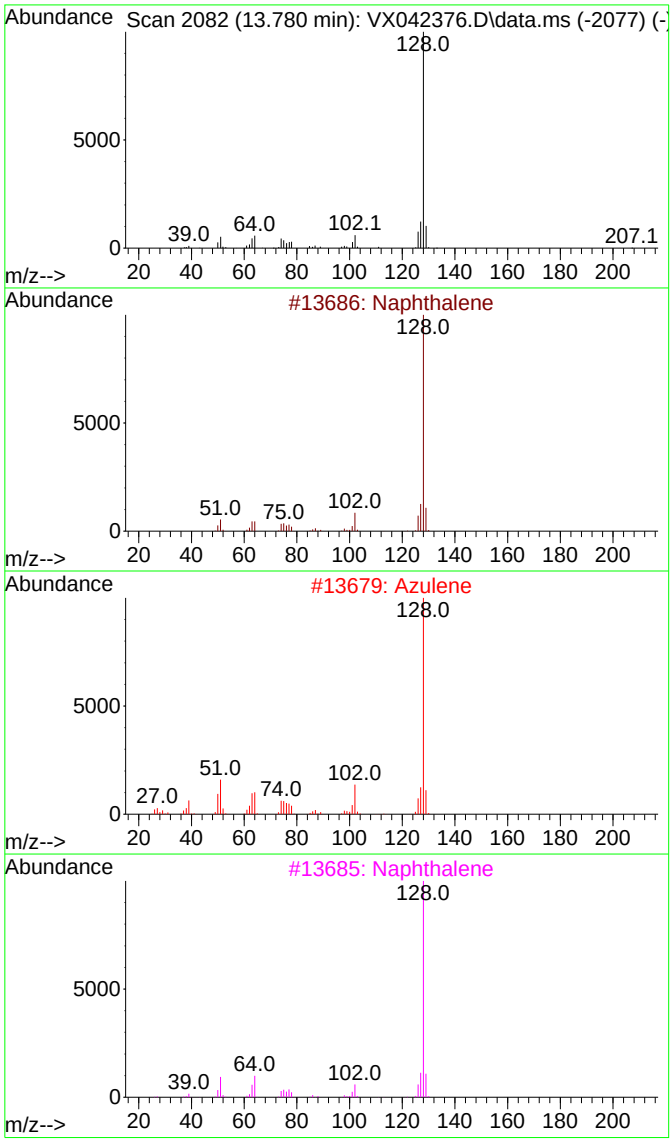
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

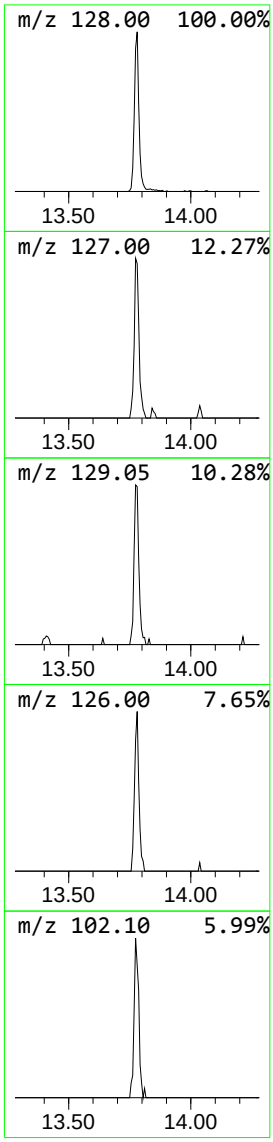
****

Peak Number 5 Azulene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	7.48 ug/L	37527	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	Naphthalene	128	C10H8	000091-20-3	91
4	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
5	Naphthalene	128	C10H8	000091-20-3	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

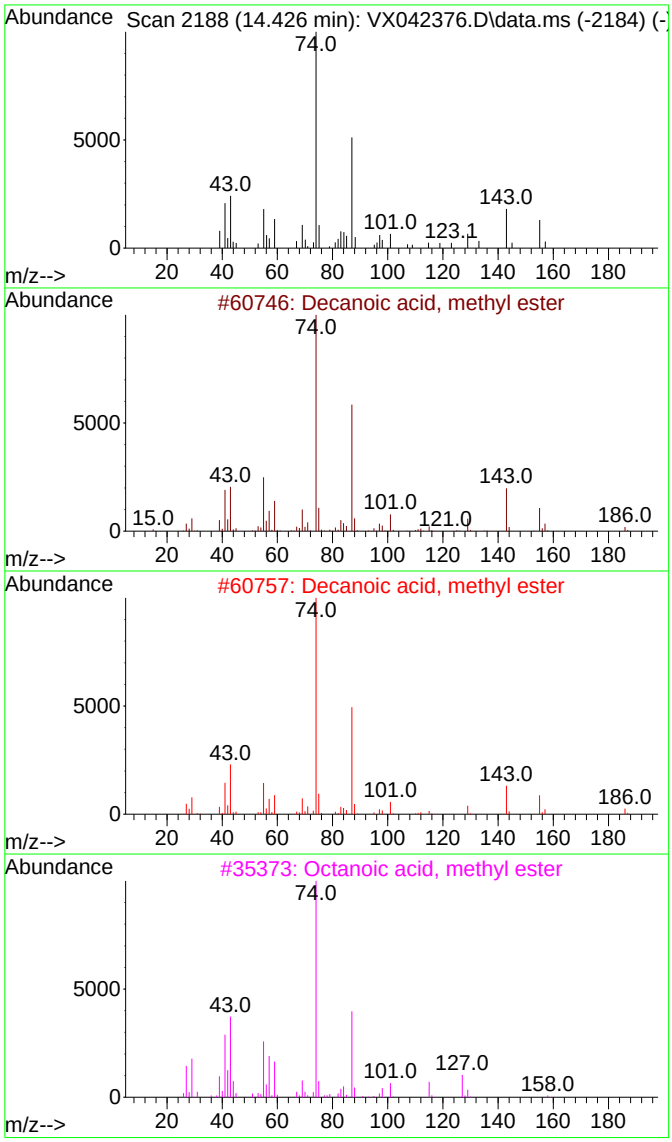
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

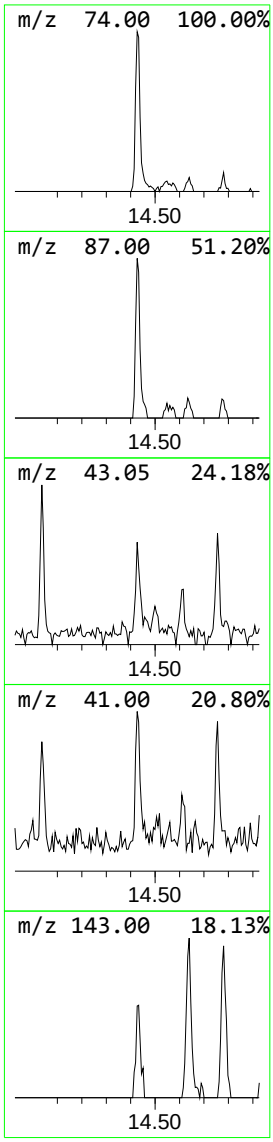
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Decanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	3.62 ug/L	18184	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	90
2	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	83
3	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	72
4	Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	72
5	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

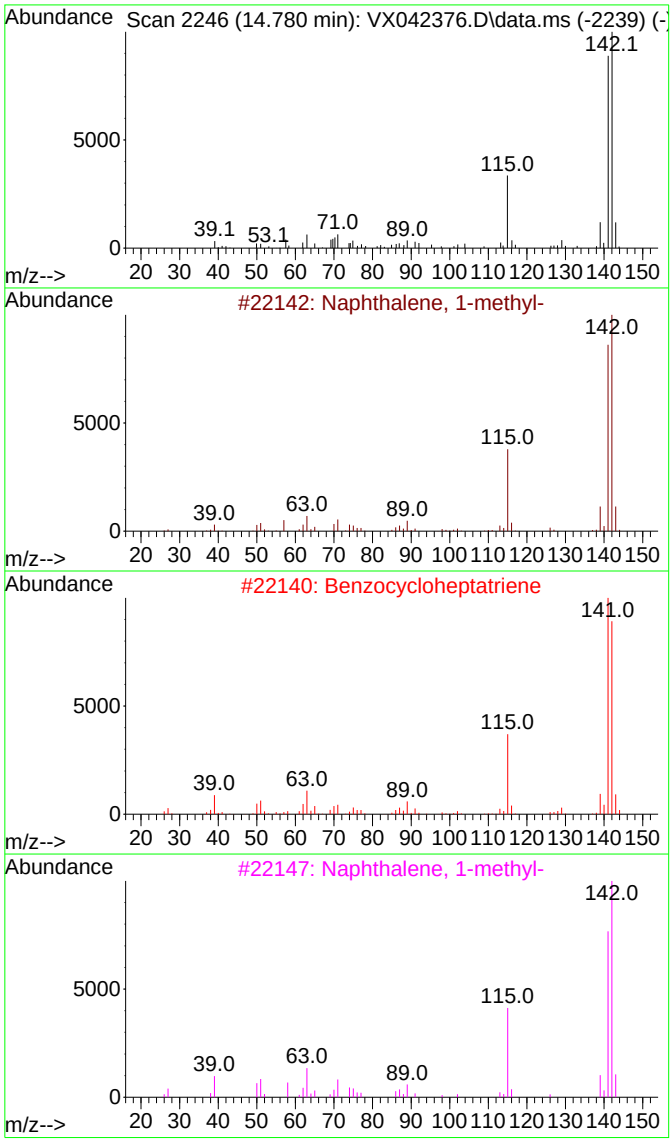
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

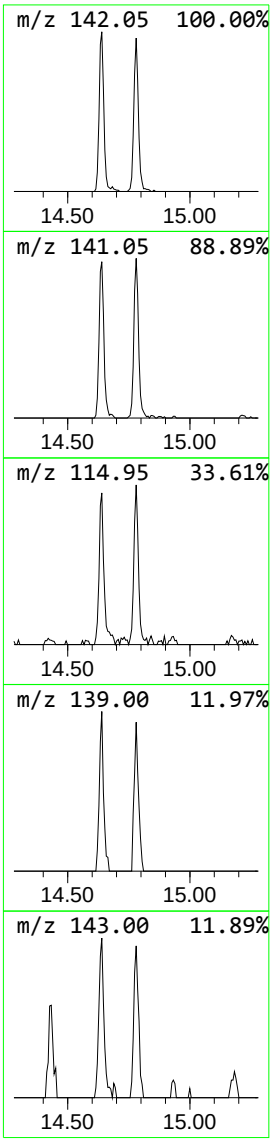
****

Peak Number 8 Benzocycloheptatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	8.02 ug/L	40237	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Benzocycloheptatriene	142	C11H10	000264-09-5	94
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	93
4	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	93
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

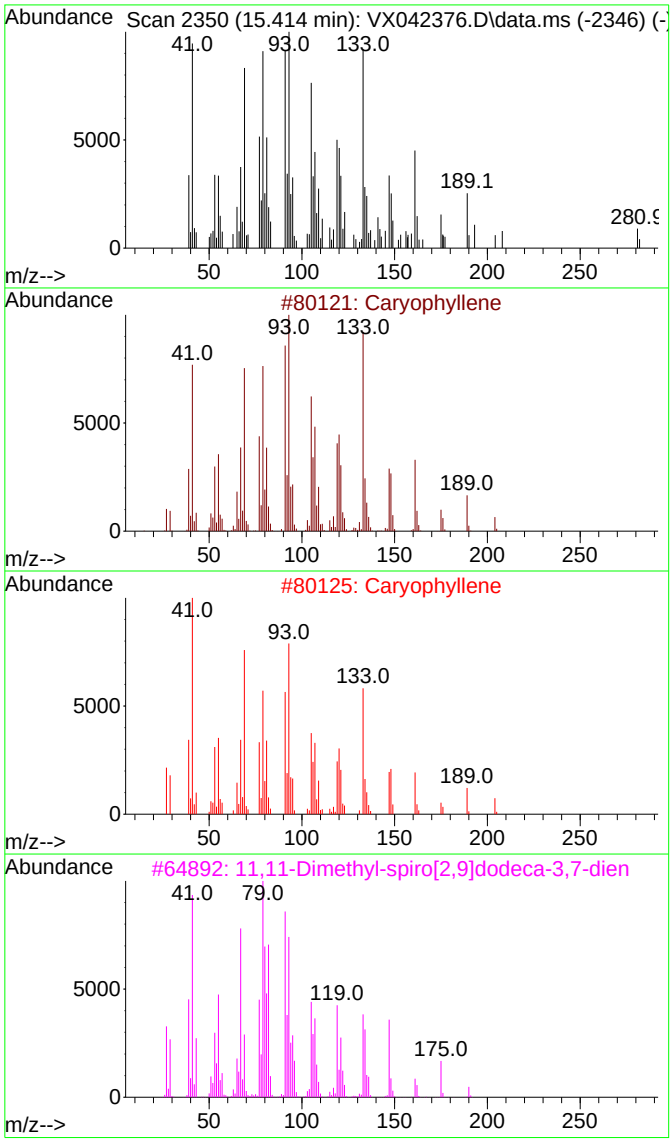
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

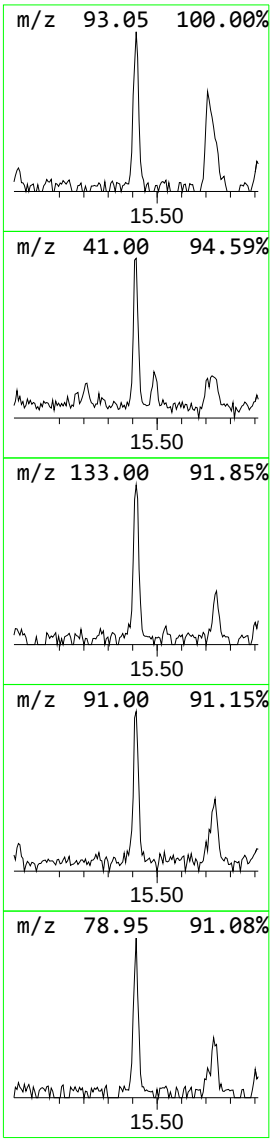
****

Peak Number 9 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.414	8.60 ug/L	43130	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Caryophyllene	204	C15H24	000087-44-5	93
3	11,11-Dimethyl-spiro[2,9]dodeca-...	190	C14H22	1000062-28-4	89
4	Caryophyllene	204	C15H24	000087-44-5	87
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

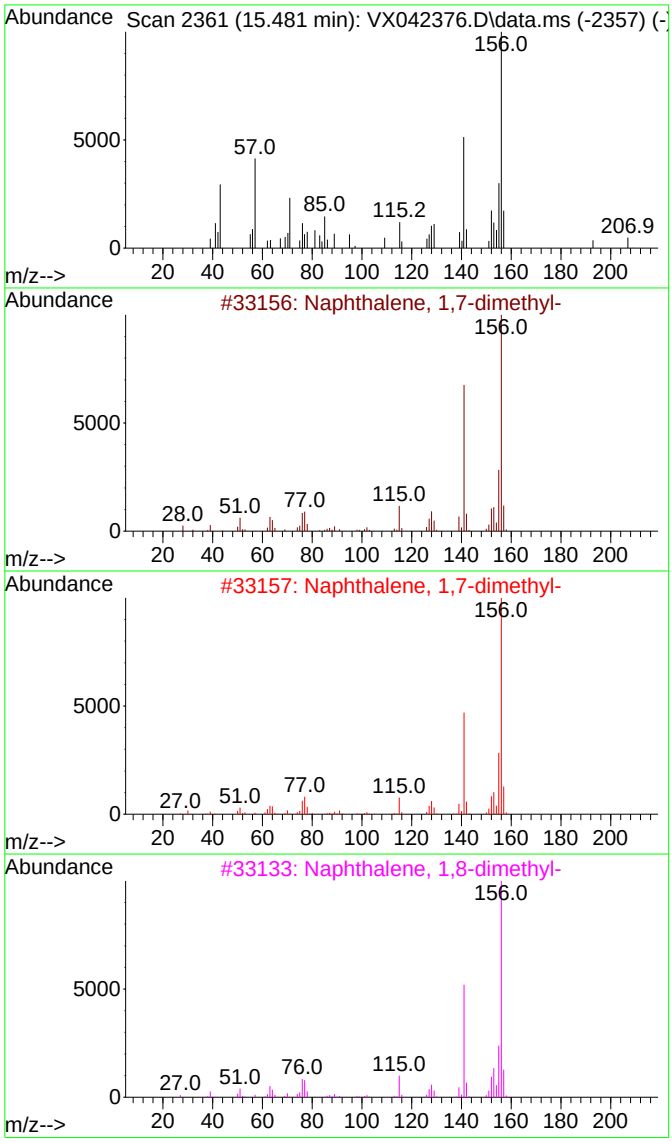
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

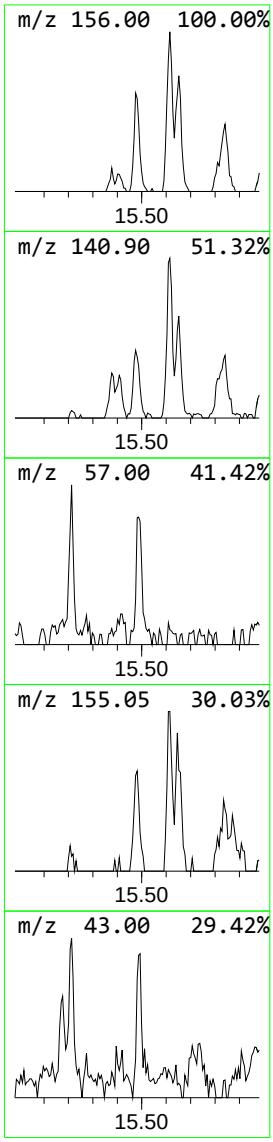
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,7-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	2.92 ug/L	14660	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	94
3	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	94
4	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

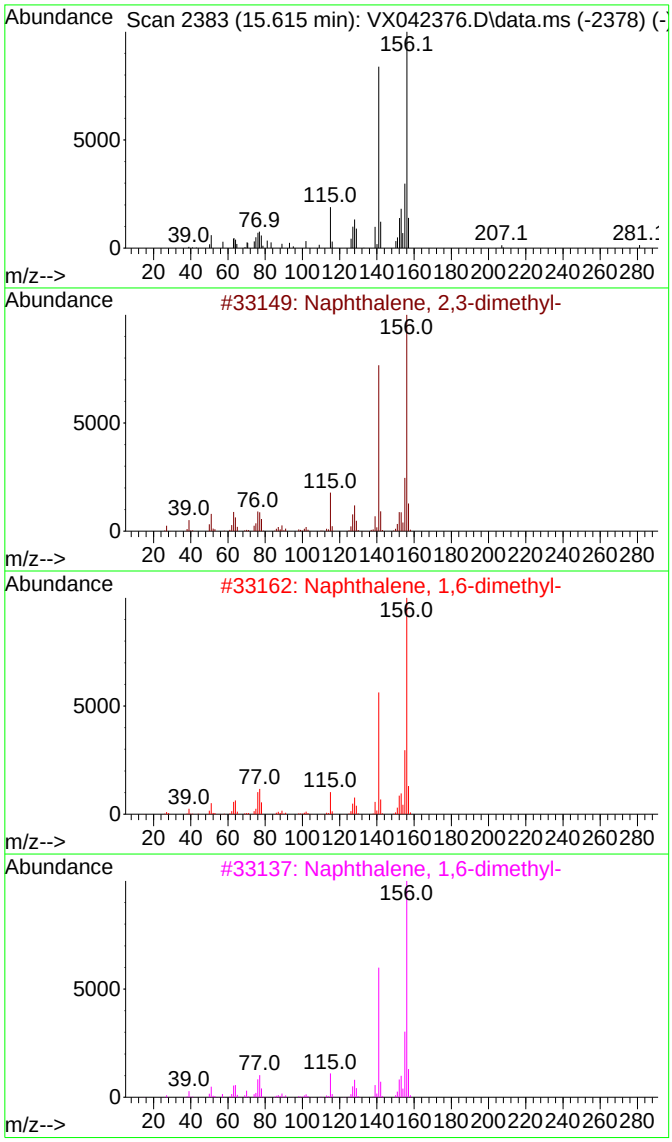
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

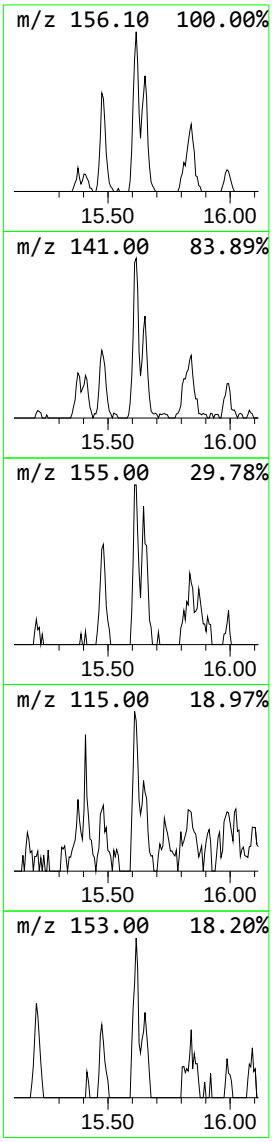
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Naphthalene, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	4.11 ug/L	20621	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
5	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

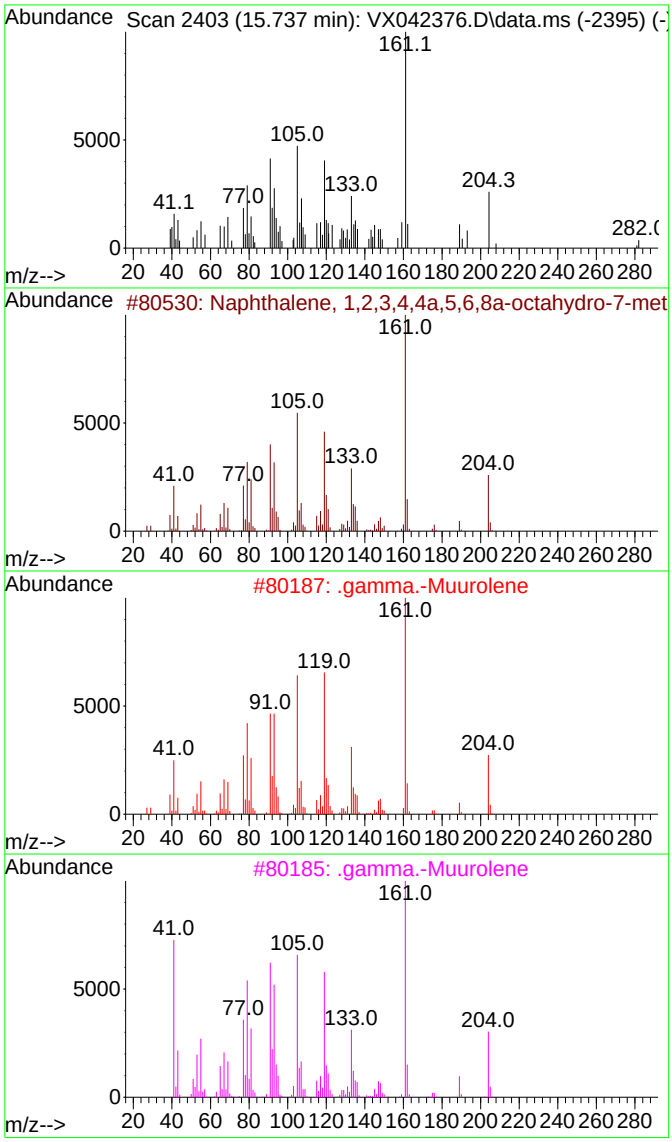
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

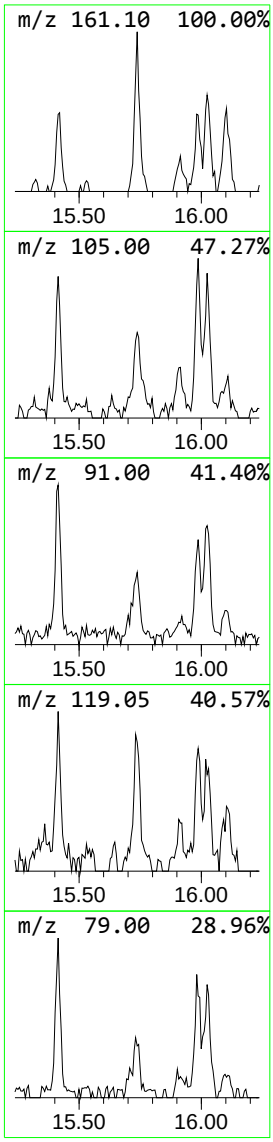
****

Peak Number 12 .gamma.-Muurolene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.737	6.34 ug/L	31822	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	039029-41-9	98
2	.gamma.-Muurolene	204	C15H24	030021-74-0	95
3	.gamma.-Muurolene	204	C15H24	030021-74-0	95
4	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	95
5	.gamma.-Muurolene	204	C15H24	030021-74-0	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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

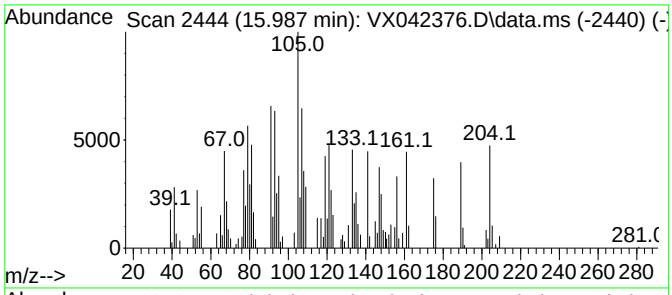
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

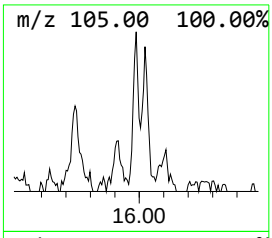
****

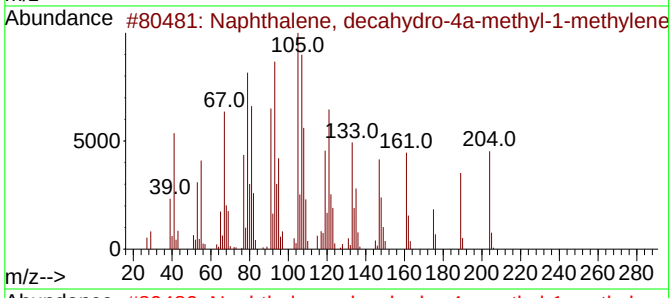
Peak Number 13 .beta.-Humulene Concentration Rank 8

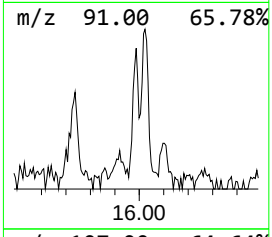
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.987	6.46 ug/L	32420	1,4-Dichlorobenzene-d4	12.024

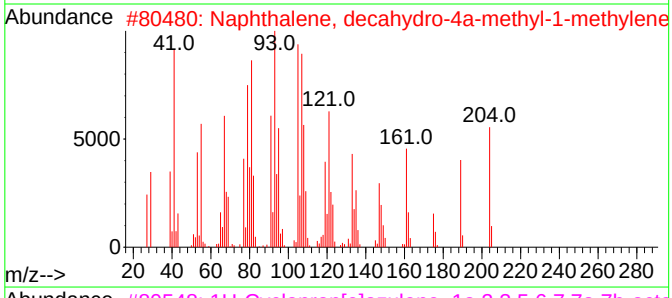
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	99
2	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	92
3	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	91
4	.beta.-Humulene	204	C15H24	000116-04-1	91
5	(-)-Aristolene	204	C15H24	006831-16-9	86

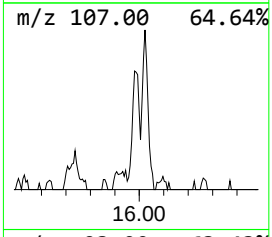


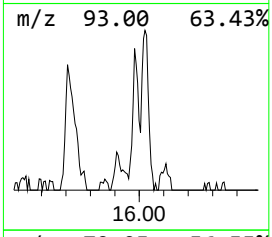


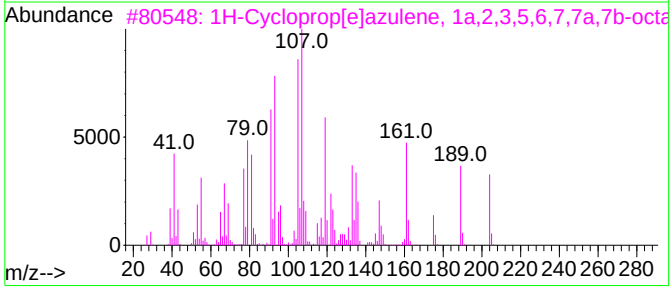


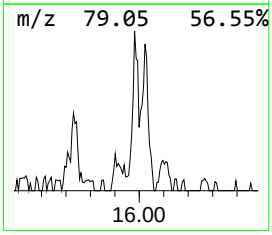












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

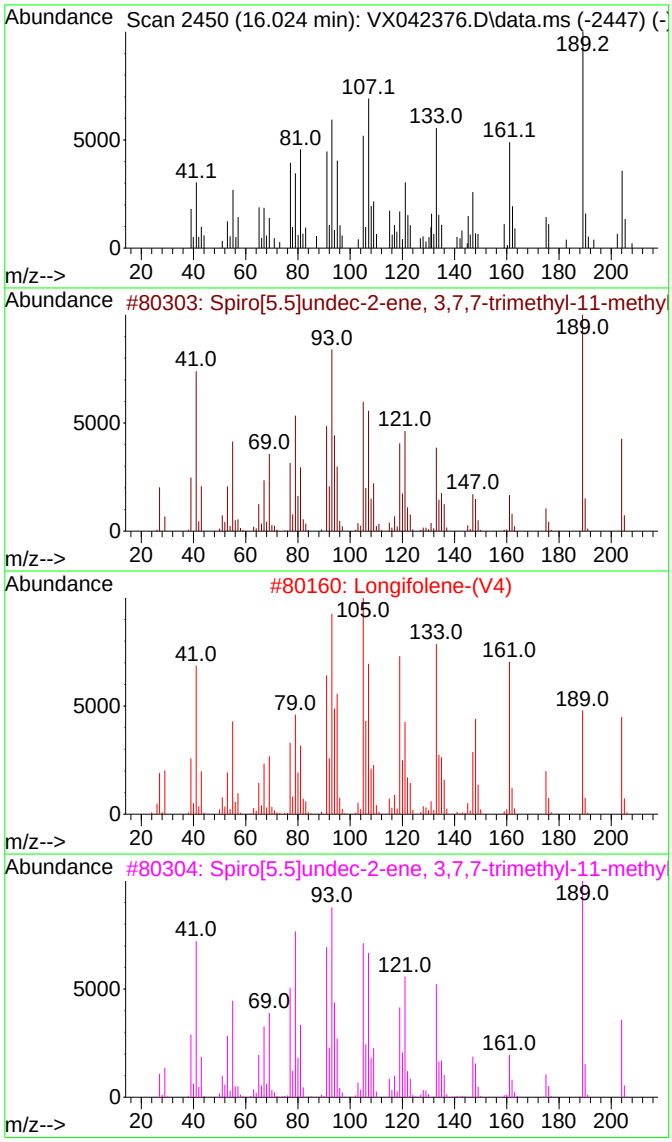
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

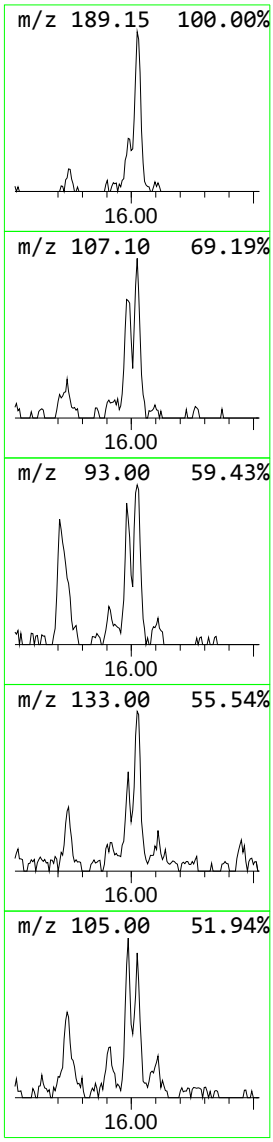
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Spiro[5.5]undec-2-ene, 3,7,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.024	9.19 ug/L	46129	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	76
2	Longifolene-(V4)	204	C15H24	061262-67-7	58
3	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	52
4	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	50
5	.gamma.-Neoclovene	204	C15H24	1000156-11-7	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042376.D
Acq On : 18 Jul 2024 17:47
Operator : JC/MD
Sample : P3215-14ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D31ME

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
unknown-01	1.258	9.3	ug/L	39370	1	6.757	211282	50.0
(DEL) Alkane: S...	11.476	2.5	ug/L	12706	3	12.024	250898	50.0
(DEL) Alkane: S...	13.268	2.9	ug/L	14722	3	12.024	250898	50.0
Azulene	13.780	7.5	ug/L	37527	3	12.024	250898	50.0
Decanoic acid, ...	14.426	3.6	ug/L	18184	3	12.024	250898	50.0
Benzocyclohepta...	14.780	8.0	ug/L	40237	3	12.024	250898	50.0
Caryophyllene	15.414	8.6	ug/L	43130	3	12.024	250898	50.0
Naphthalene, 1,...	15.481	2.9	ug/L	14660	3	12.024	250898	50.0
Naphthalene, 2,...	15.615	4.1	ug/L	20621	3	12.024	250898	50.0
.gamma.-Muurolene	15.737	6.3	ug/L	31822	3	12.024	250898	50.0
.beta.-Humulene	15.987	6.5	ug/L	32420	3	12.024	250898	50.0
Spiro[5.5]undec...	16.024	9.2	ug/L	46129	3	12.024	250898	50.0