LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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: VX042369.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	40	rBV2	17482	29820	5.53%	0.878%
2	1.374	43	47	48	rBV	4889	6149	1.14%	0.181%
3	1.538	71	74	76	rBV2	1766	2505	0.46%	0.074%
4	2.276	190	195	205	rBV	24124	40543	7.52%	1.194%
5	2.721	262	268	273	rBV	7025	14534	2.70%	0.428%
6	2.947	303	305	309	rVB3	432	575	0.11%	0.017%
7	3.075	322	326	330	rVB2	345	434	0.08%	0.013%
8	3.593	405	411	423	rVV4	1783	5090	0.94%	0.150%
9	3.934	464	467	470	rBV2	161	198	0.04%	0.006%
10	4.501	550	560	579	rBV2	9752	38660	7.17%	1.139%
11	5.056	640	651	667	rBV2	20767	66271	12.30%	1.952%
12	5.556	725	733	740	rBV5	841	2597	0.48%	0.076%
13	5.964	789	800	816	rBV3	59843	172830	32.07%	5.091%
14	6.196	834	838	840	rBV2	161	188	0.03%	0.006%
15	6.300	854	855	858	rBV	160	179	0.03%	0.005%
16	6.373	865	867	868	rBV2	284	196	0.04%	0.006%
17	6.538	892	894	897	rVB3	146	188	0.03%	0.006%
18	6.666	912	915	917	rBV3	218	333	0.06%	0.010%
19	6.757	921	930	946	rBV	189057	449462	83.40%	13.239%
20	7.129	984	991	997	rBV3	1100	2390	0.44%	0.070%
21	7.220	1002	1006	1008	rBV2	399	555	0.10%	0.016%
22	7.306	1012	1020	1030	rBV2	33723	76962	14.28%	2.267%
23	7.976	1127	1130	1132	rVV2	352	310	0.06%	0.009%
24	8.330	1181	1188	1202	rBV	17319	31217	5.79%	0.919%
25	8.507	1215	1217	1220	rBV2	124	173	0.03%	0.005%
26	8.647	1234	1240	1249	rBV	82009	135174	25.08%	3.981%
27	8.915	1280	1284	1286	rBV2	297	384	0.07%	0.011%
28	8.958	1286	1291	1299	rBV	10824	18480	3.43%	0.544%
29	9.275	1340	1343	1347	rBV3	1293	1811	0.34%	0.053%
30	9.397	1358	1363	1377	rBV2	35755	81527	15.13%	2.401%
31	9.811	1429	1431	1434	rBV	221	213	0.04%	0.006%
32	10.055	1465	1471	1486	rBV	370959	528387	98.05%	15.563%
33	10.311	1508	1513	1517	rBV3	1317	2031	0.38%	0.060%
34	10.360	1518	1521	1526	rVB4	1029	1203	0.22%	0.035%
35	10.470	1537	1539	1541	rVB	194	173	0.03%	0.005%
36	10.506	1541	1545	1546	rBV2	139	213	0.04%	0.006%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
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Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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	10.592	1556	1559	1560	rBV	189	198	0.04%	0.006%
38	10.640	1565	1567	1574	rVB3	635	1117	0.21%	0.033%
39	10.689	1574	1575	1579	rBV2	190	219	0.04%	0.006%
40	10.781	1587	1590	1592	rBV2	447	481	0.09%	0.014%
41	10.823	1593	1597	1599	rVB3	745	1035	0.19%	0.030%
42	10.860	1599	1603	1604	rBV	170	171	0.03%	0.005%
43	10.897	1606	1609	1611	rVV2	437	546	0.10%	0.016%
44	10.945	1612	1617	1625	rVV2	2500	4047	0.75%	0.119%
45	11.195	1650	1658	1665	rBV	74406	103362	19.18%	3.044%
46	11.311	1673	1677	1682	rBV3	943	1343	0.25%	0.040%
47	11.476	1698	1704	1711	rBV4	3883	6386	1.19%	0.188%
48	11.652	1731	1733	1735	rVB	246	202	0.04%	0.006%
49	11.701	1735	1741	1743	rBV3	1402	2048	0.38%	0.060%
50	11.732	1744	1746	1748	rVV2	3703	4400	0.82%	0.130%
51	11.762	1749	1751	1758	rVB2	8804	10013	1.86%	0.295%
52	11.823	1758	1761	1764	rBV2	3414	3667	0.68%	0.108%
53	11.939	1776	1780	1783	rBV4	1872	2572	0.48%	0.076%
54	11.976	1783	1786	1788	rBV2	446	609	0.11%	0.018%
55	12.024	1788	1794	1804	rBV	411089	538898	100.00%	15.873%
56	12.244	1827	1830	1835	rVB3	1412	1691	0.31%	0.050%
57	12.317	1838	1842	1854	rVB	107465	145571	27.01%	4.288%
58	12.421	1854	1859	1863	rBV3	4955	7287	1.35%	0.215%
59	12.616	1888	1891	1896	rVB3	428	726	0.13%	0.021%
60	12.701	1899	1905	1910	rBV3	429	800	0.15%	0.024%
61	12.768	1910	1916	1919	rVB3	681	978	0.18%	0.029%
62	12.860	1928	1931	1939	rBV5	1491	3281	0.61%	0.097%
63	12.975	1946	1950	1952	rVB2	486	441	0.08%	0.013%
64	13.170	1980	1982	1987	rVV3	347	473	0.09%	0.014%
65	13.268	1994	1998	2000	rBV3	1600	1801	0.33%	0.053%
66	13.292	2000	2002	2007	rVB	1285	1226	0.23%	0.036%
67	13.408	2012	2021	2026	rBV4	1233	2249	0.42%	0.066%
68	13.500	2035	2036	2041	rVB2	167	220	0.04%	0.006%
69	13.555	2041	2045	2048	rVB3	329	344	0.06%	0.010%
70	13.591	2048	2051	2057	rBV2	503	811	0.15%	0.024%
71	13.640	2057	2059	2062	rBV2	240	215	0.04%	0.006%
72	13.689	2062	2067	2071	rBV5	684	1183	0.22%	0.035%
73	13.725	2071	2073	2074	rBV	185	182	0.03%	0.005%
74	13.774	2077	2081	2090	rBV	29618	40573	7.53%	1.195%
75	13.872	2095	2097	2105	rVB2	544	789	0.15%	0.023%
76	14.036	2122	2124	2128	rVB4	1281	1446	0.27%	0.043%

LSC Area Percent Report

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Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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	14.128	2136	2139	2145	rVB2	802	1170	0.22%	0.034%
78	14.182	2145	2148	2149	rBV3	215	272	0.05%	0.008%
79	14.219	2151	2154	2157	rVV2	290	417	0.08%	0.012%
80	14.371	2177	2179	2182	rVB2	266	229	0.04%	0.007%
81	14.426	2185	2188	2192	rBV3	1235	1741	0.32%	0.051%
82	14.512	2201	2202	2203	rBV	373	205	0.04%	0.006%
83	14.609	2216	2218	2219	rBV2	630	477	0.09%	0.014%
84	14.640	2219	2223	2228	rVB	14690	18375	3.41%	0.541%
85	14.780	2242	2246	2249	rBV	11855	13324	2.47%	0.392%
86	14.823	2249	2253	2258	rVB2	13050	17136	3.18%	0.505%
87	14.896	2261	2265	2269	rBV2	4662	5992	1.11%	0.176%
88	15.207	2313	2316	2320	rVB2	4026	5279	0.98%	0.155%
89	15.255	2322	2324	2327	rBV4	1172	1249	0.23%	0.037%
90	15.316	2331	2334	2339	rBV4	2774	4515	0.84%	0.133%
91	15.377	2341	2344	2348	rVB4	2638	3264	0.61%	0.096%
92	15.481	2356	2361	2369	rVB3	6814	11969	2.22%	0.353%
93	15.585	2373	2378	2380	rBV2	8602	13167	2.44%	0.388%
94	15.658	2386	2390	2396	rVB3	37876	60307	11.19%	1.776%
95	15.743	2399	2404	2409	rVB2	32273	45720	8.48%	1.347%
96	15.871	2419	2425	2435	rVB	308224	504660	93.65%	14.865%
97	16.048	2451	2454	2458	rVB3	4153	4916	0.91%	0.145%
98	16.280	2485	2492	2495	rBV2	20942	37320	6.93%	1.099%
99	16.322	2496	2499	2508	rVB2	20309	36557	6.78%	1.077%
100	16.456	2519	2521	2526	rBV3	873	1248	0.23%	0.037%

Sum of corrected areas: 3395065

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
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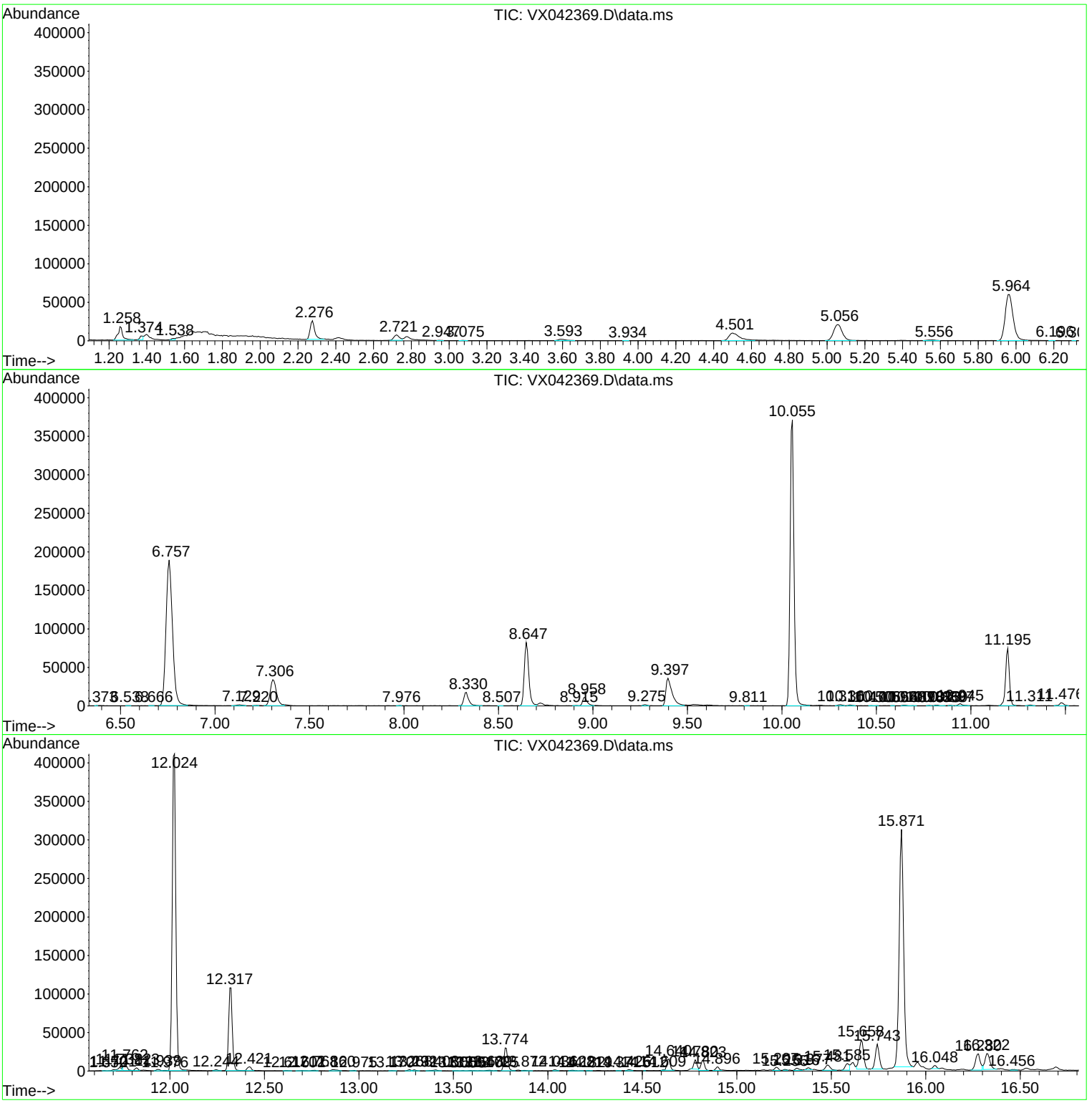
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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 : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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

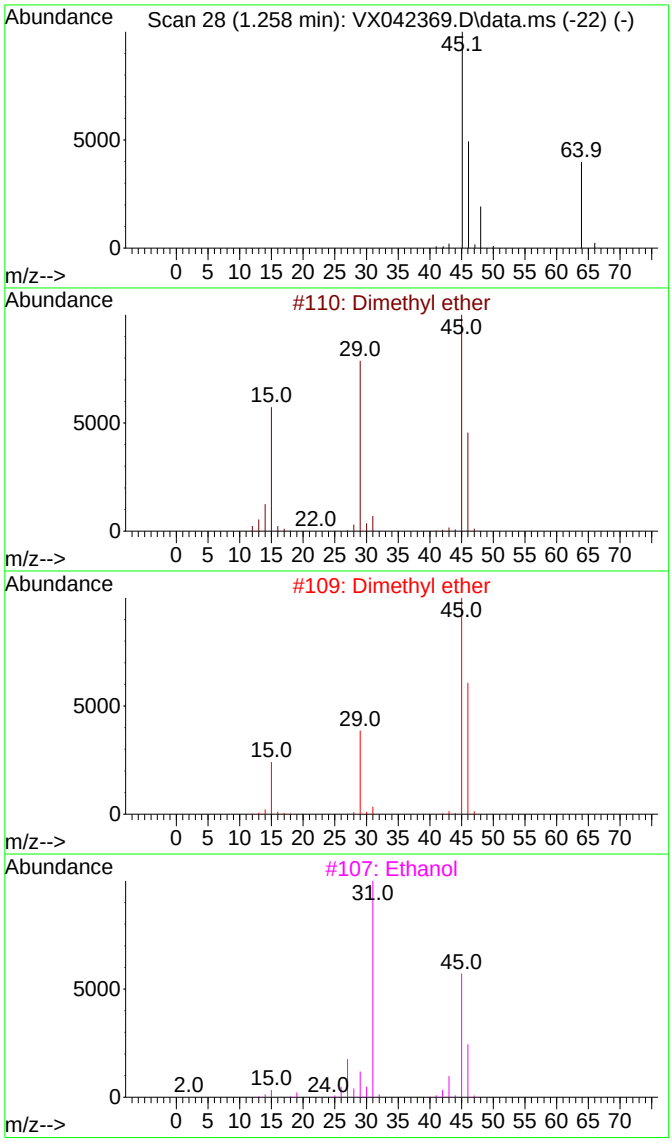
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

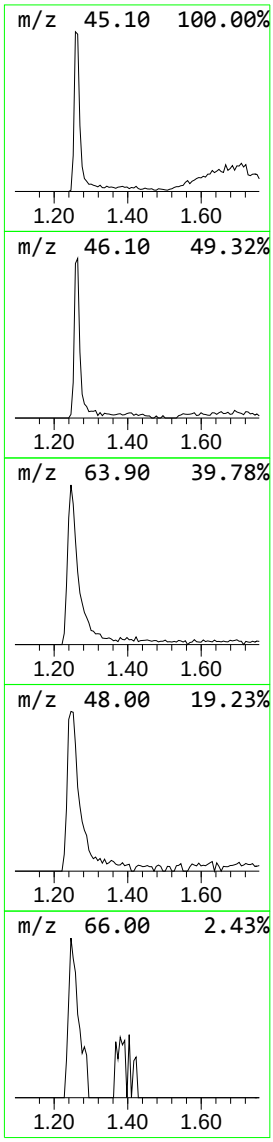
****

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	3.32 ug/L	29820	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	16
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Ethanol	46	C2H6O	000064-17-5	7
4	Ethanol	46	C2H6O	000064-17-5	7
5	Ethanol	46	C2H6O	000064-17-5	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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

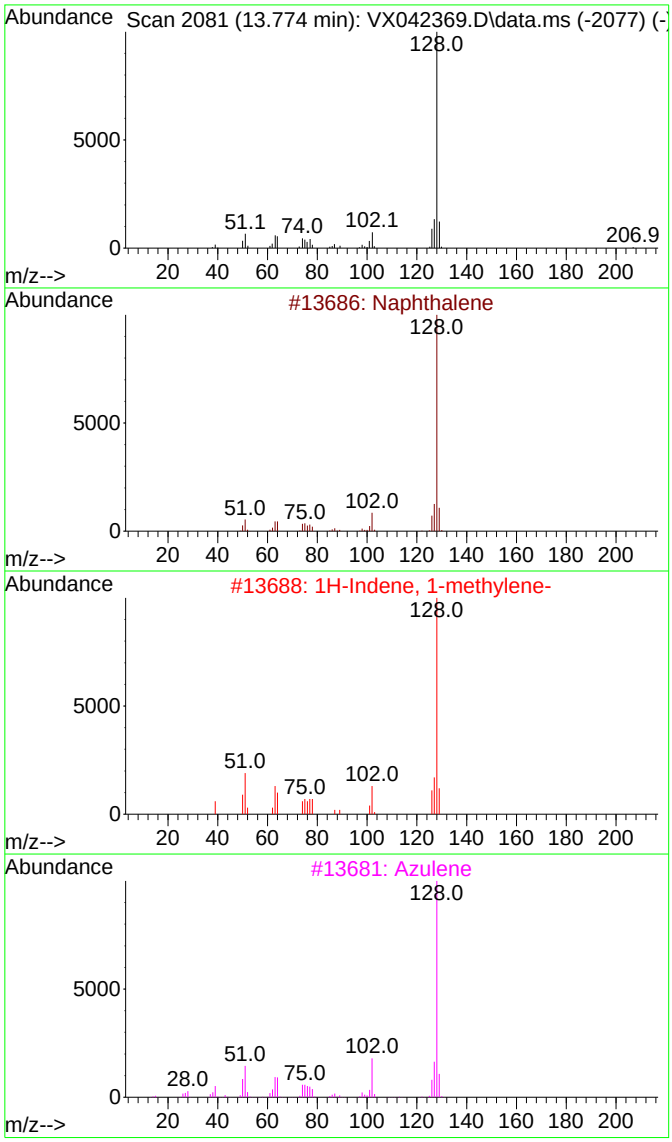
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

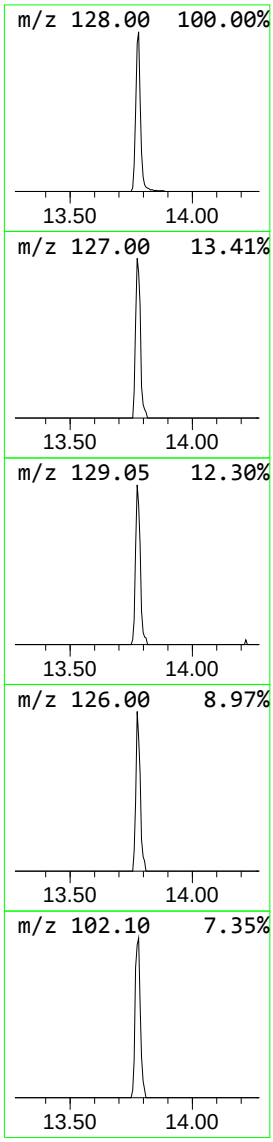
****

Peak Number 3 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	3.76 ug/L	40573	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	94
3	Azulene	128	C10H8	000275-51-4	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Naphthalene	128	C10H8	000091-20-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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

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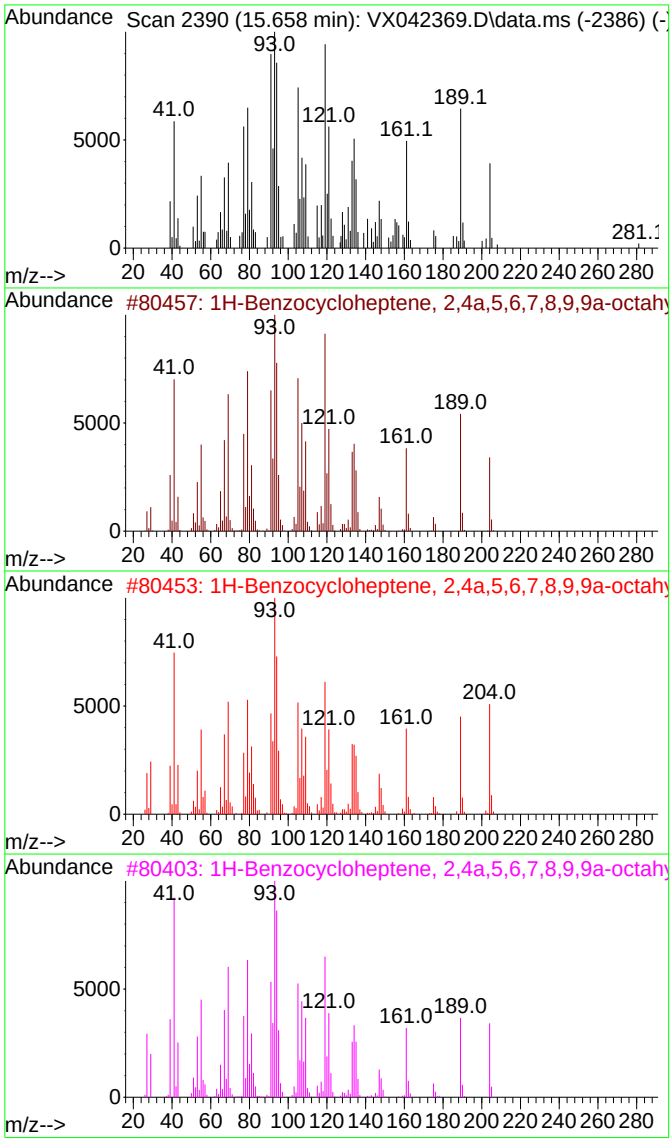
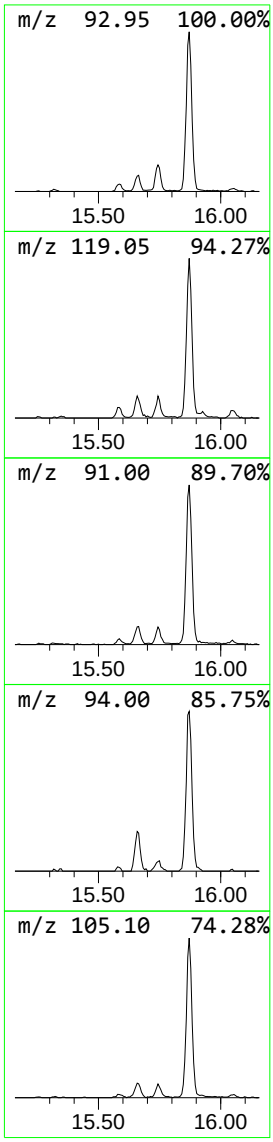
Peak Number 4 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.658	5.60 ug/L	60307	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	99
2	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	99
3	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	080923-88-2	99
4	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	99
5	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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

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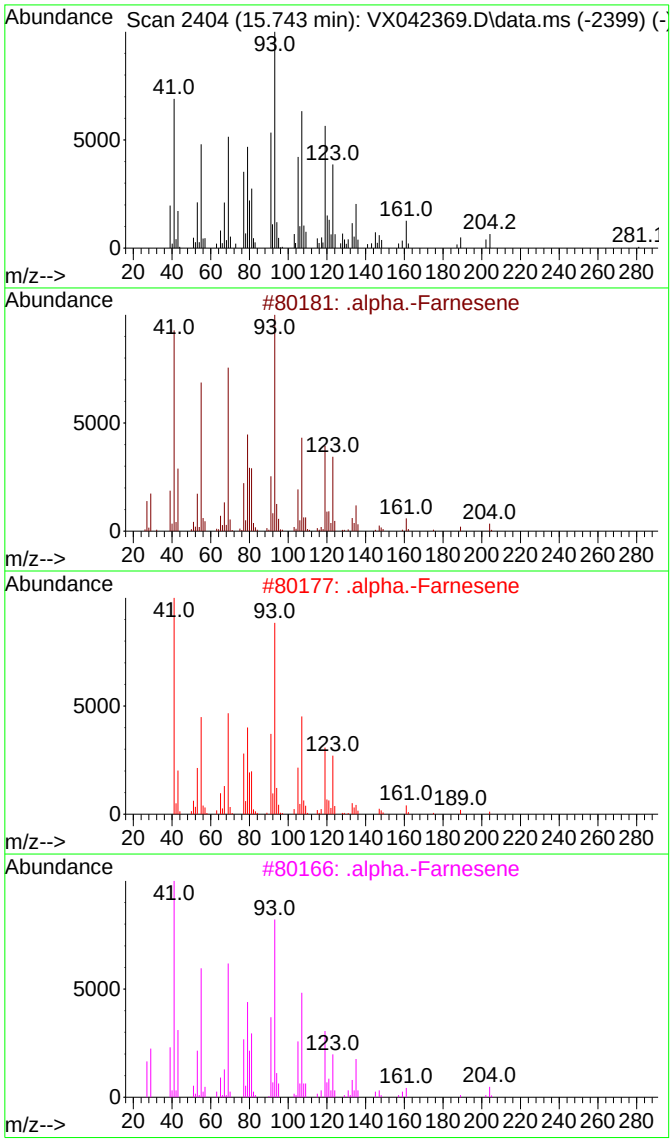
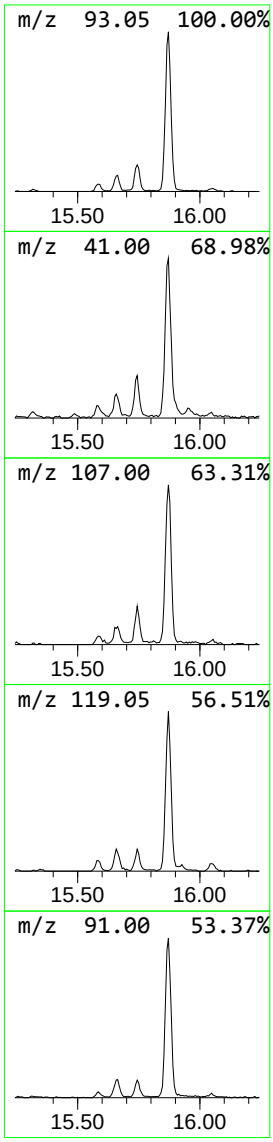
Peak Number 5 .alpha.-Farnesene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.743	4.24 ug/L	45720	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Farnesene	204	C15H24	000502-61-4	96
2	.alpha.-Farnesene	204	C15H24	000502-61-4	95
3	.alpha.-Farnesene	204	C15H24	000502-61-4	91
4	.alpha.-Farnesene	204	C15H24	000502-61-4	87
5	(Z)-1-Methyl-4-(6-methylhept-5-e...	204	C15H24	013062-00-5	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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

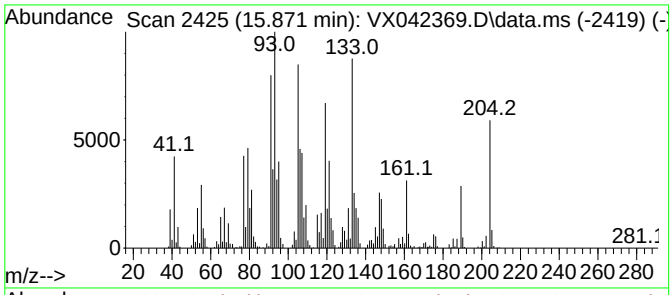
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

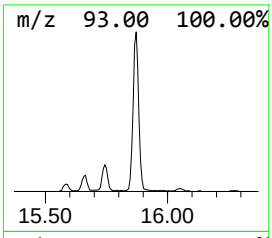
****

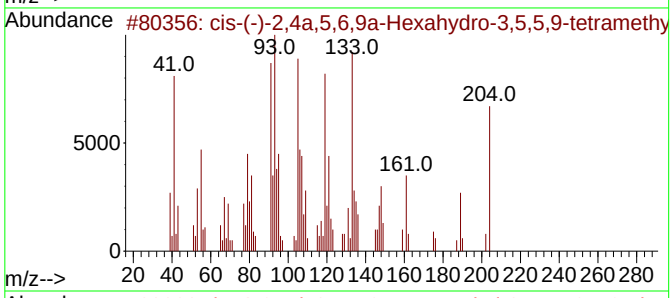
Peak Number 6 cis-Thujopsene Concentration Rank 1

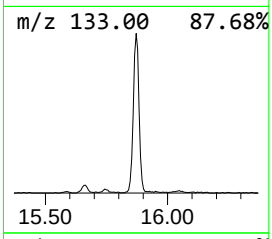
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.871	46.82 ug/L	504660	1,4-Dichlorobenzene-d4	12.024

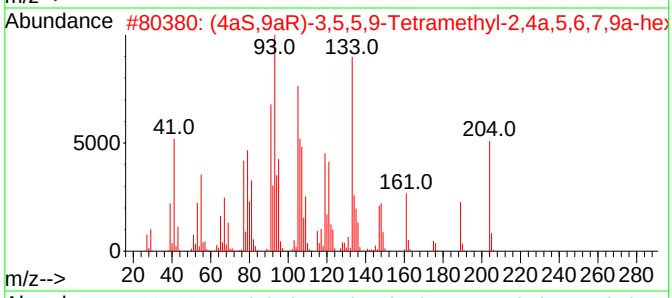
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	99
2	(4aS,9aR)-3,5,5,9-Tetramethyl-2,...	204	C15H24	053111-25-4	99
3	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	70
4	cis-Thujopsene	204	C15H24	000470-40-6	64
5	Alloaromadendrene	204	C15H24	025246-27-9	62

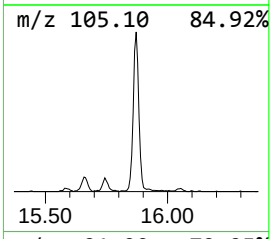


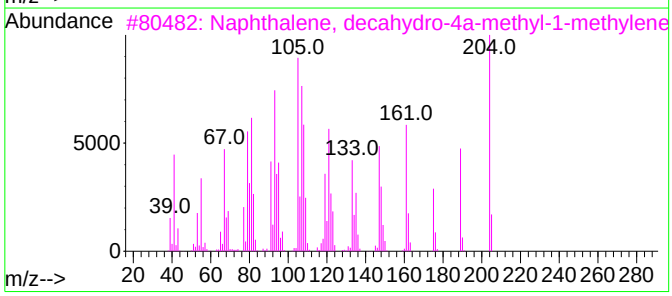


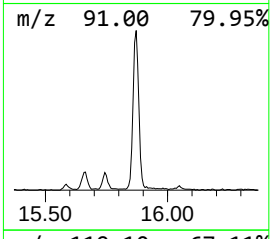


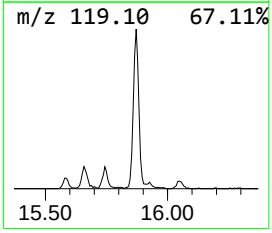












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

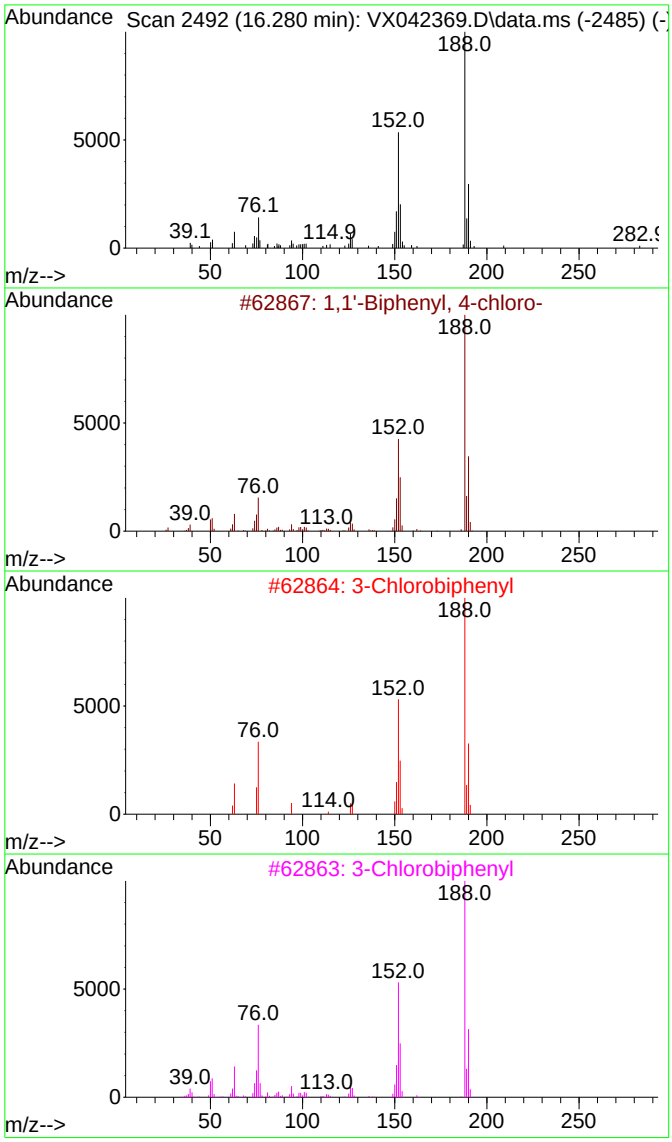
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

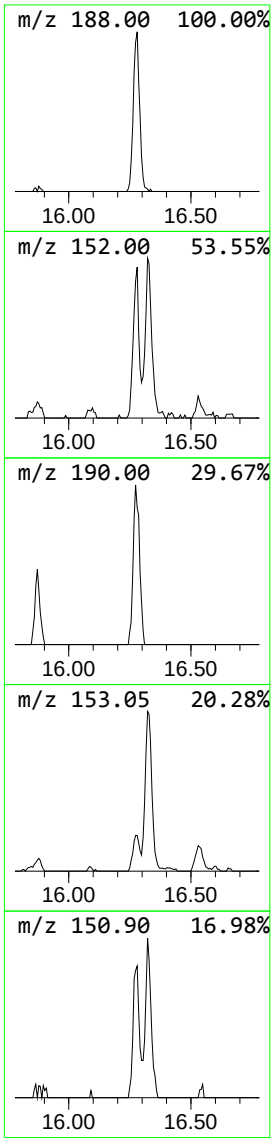
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,1'-Biphenyl, 4-chloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.280	3.46 ug/L	37320	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96
2	3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
3	3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	96
4	1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	96
5	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	96





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

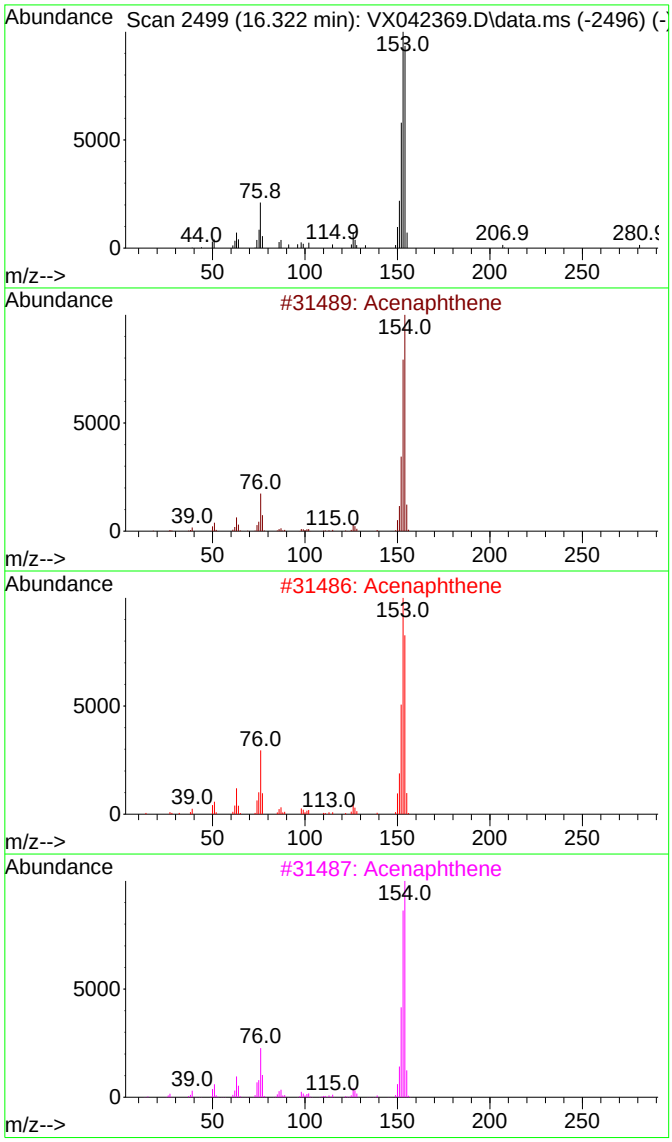
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

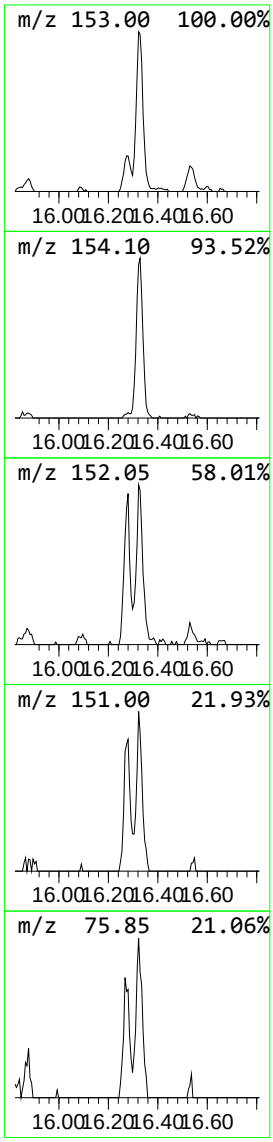
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2-ethenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	3.39 ug/L	36557	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	68
2	Acenaphthene	154	C12H10	000083-32-9	62
3	Acenaphthene	154	C12H10	000083-32-9	59
4	Acenaphthene	154	C12H10	000083-32-9	58
5	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042369.D
Acq On : 18 Jul 2024 15:08
Operator : JC/MD
Sample : P3215-04ME
Misc : 5.29g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C02ME

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	3.3	ug/L	29820	1	6.757	449462	50.0
Azulene	13.774	3.8	ug/L	40573	3	12.024	538898	50.0
unknown-02	15.658	5.6	ug/L	60307	3	12.024	538898	50.0
.alpha.-Farnesene	15.743	4.2	ug/L	45720	3	12.024	538898	50.0
cis-Thujopsene	15.871	46.8	ug/L	504660	3	12.024	538898	50.0
1,1'-Biphenyl, ...	16.280	3.5	ug/L	37320	3	12.024	538898	50.0
Naphthalene, 2-...	16.322	3.4	ug/L	36557	3	12.024	538898	50.0