LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
Data File : VX042374.D
Acq On : 18 Jul 2024 17:00
Operator : JC/MD
Sample : P3215-11ME
Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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: VX042374.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	10	rBV	327	195	0.04%	0.004%
2	1.258	22	28	36	rBV2	16327	29303	5.48%	0.632%
3	1.374	43	47	49	rBV	14750	23770	4.45%	0.513%
4	1.538	71	74	75	rBV	1527	1712	0.32%	0.037%
5	1.648	89	92	95	rBV2	8337	14596	2.73%	0.315%
6	2.276	189	195	212	rBV	73381	142250	26.63%	3.069%
7	2.483	227	229	232	rVB2	416	309	0.06%	0.007%
8	2.776	271	277	284	rBV2	3857	8154	1.53%	0.176%
9	2.892	294	296	300	rVB2	215	240	0.04%	0.005%
10	2.941	302	304	307	rBV3	261	363	0.07%	0.008%
11	3.069	322	325	327	rVV	130	170	0.03%	0.004%
12	3.416	378	382	386	rBV2	336	426	0.08%	0.009%
13	3.593	408	411	414	rVV2	122	170	0.03%	0.004%
14	4.056	482	487	488	rBV	203	190	0.04%	0.004%
15	4.105	494	495	502	rBV2	95	170	0.03%	0.004%
16	4.495	548	559	580	rBV	33047	125217	23.44%	2.702%
17	4.812	609	611	615	rVB2	390	425	0.08%	0.009%
18	4.971	636	637	639	rBV	177	177	0.03%	0.004%
19	5.056	639	651	668	rVV2	67762	208944	39.11%	4.508%
20	5.276	684	687	689	rVV	181	268	0.05%	0.006%
21	5.373	700	703	704	rVV3	350	332	0.06%	0.007%
22	5.391	704	706	714	rVV	569	966	0.18%	0.021%
23	5.550	727	732	733	rBV3	570	754	0.14%	0.016%
24	5.696	752	756	758	rVB2	183	220	0.04%	0.005%
25	5.964	789	800	820	rBV2	187836	534240	100.00%	11.527%
26	6.385	861	869	876	rBV5	1346	4314	0.81%	0.093%
27	6.757	920	930	949	rBV	166328	397684	74.44%	8.581%
28	7.117	983	989	990	rBV3	998	1721	0.32%	0.037%
29	7.220	999	1006	1012	rBV4	2287	5180	0.97%	0.112%
30	7.306	1012	1020	1032	rBV	108118	237416	44.44%	5.123%
31	7.897	1116	1117	1122	rBV2	96	181	0.03%	0.004%
32	7.970	1122	1129	1134	rVV6	950	1917	0.36%	0.041%
33	8.251	1171	1175	1178	rBV2	315	418	0.08%	0.009%
34	8.324	1182	1187	1198	rBV	57553	100332	18.78%	2.165%
35	8.525	1218	1220	1223	rVB2	255	252	0.05%	0.005%
36	8.647	1234	1240	1255	rBV	268532	419387	78.50%	9.049%

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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	8.763	1255	1259	1267	rVB2	2081	4097	0.77%	0.088%
38	8.872	1275	1277	1282	rVB3	242	338	0.06%	0.007%
39	8.952	1284	1290	1304	rBV	42704	66388	12.43%	1.432%
40	9.049	1304	1306	1309	rVV2	275	305	0.06%	0.007%
41	9.116	1313	1317	1321	rBV3	727	868	0.16%	0.019%
42	9.275	1340	1343	1350	rBV	362	507	0.09%	0.011%
43	9.391	1357	1362	1384	rBV	132722	277813	52.00%	5.994%
44	9.616	1395	1399	1403	rVV4	863	1205	0.23%	0.026%
45	9.647	1403	1404	1409	rVB2	339	324	0.06%	0.007%
46	9.775	1423	1425	1428	rVB2	196	207	0.04%	0.004%
47	9.830	1428	1434	1438	rVB3	838	1212	0.23%	0.026%
48	10.055	1465	1471	1485	rBV	331255	460123	86.13%	9.928%
49	10.171	1488	1490	1493	rVB3	450	393	0.07%	0.008%
50	10.275	1503	1507	1510	rBV3	847	1410	0.26%	0.030%
51	10.317	1510	1514	1518	rVB4	1365	2228	0.42%	0.048%
52	10.348	1518	1519	1520	rBV	334	188	0.04%	0.004%
53	10.372	1520	1523	1526	rVB	339	387	0.07%	0.008%
54	10.458	1533	1537	1541	rVB2	668	680	0.13%	0.015%
55	10.531	1546	1549	1551	rBV3	560	718	0.13%	0.015%
56	10.586	1551	1558	1563	rVB7	2085	4122	0.77%	0.089%
57	10.647	1566	1568	1569	rBV	587	547	0.10%	0.012%
58	10.665	1569	1571	1577	rVB4	953	1342	0.25%	0.029%
59	10.781	1581	1590	1594	rBV2	4056	7208	1.35%	0.156%
60	10.854	1594	1602	1605	rBV6	2780	5898	1.10%	0.127%
61	10.890	1605	1608	1613	rVB2	6700	9777	1.83%	0.211%
62	10.945	1613	1617	1622	rVB4	2211	3600	0.67%	0.078%
63	11.006	1622	1627	1628	rBV2	1808	2469	0.46%	0.053%
64	11.031	1628	1631	1636	rVB	2731	3588	0.67%	0.077%
65	11.085	1636	1640	1643	rBV5	666	911	0.17%	0.020%
66	11.122	1643	1646	1650	rVB4	1439	1917	0.36%	0.041%
67	11.195	1652	1658	1667	rBV	228681	314648	58.90%	6.789%
68	11.335	1672	1681	1686	rBV8	3293	7844	1.47%	0.169%
69	11.390	1687	1690	1693	rVB5	2323	2724	0.51%	0.059%
70	11.433	1693	1697	1701	rBV3	4474	6472	1.21%	0.140%
71	11.482	1701	1705	1709	rBV4	5018	6987	1.31%	0.151%
72	11.604	1722	1725	1727	rBV3	2301	2825	0.53%	0.061%
73	11.628	1727	1729	1735	rVB3	3638	4803	0.90%	0.104%
74	11.683	1735	1738	1740	rBV4	2496	2946	0.55%	0.064%
75	11.713	1740	1743	1746	rBV3	5139	6218	1.16%	0.134%
76	11.744	1746	1748	1751	rVB3	4177	4218	0.79%	0.091%

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Misc : 5.94g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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

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Peak separation: 5

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

77	11.841	1760	1764	1766	rBV2	4146	6419	1.20%	0.139%
78	11.933	1776	1779	1783	rBV3	4640	6330	1.18%	0.137%
79	11.976	1783	1786	1789	rVB5	3262	3868	0.72%	0.083%
80	12.024	1789	1794	1805	rVB	352682	463472	86.75%	10.000%
81	12.128	1805	1811	1812	rBV6	3533	6943	1.30%	0.150%
82	12.189	1819	1821	1826	rVB4	2739	4202	0.79%	0.091%
83	12.262	1826	1833	1836	rBV7	3773	8380	1.57%	0.181%
84	12.323	1836	1843	1849	rBV	327383	446462	83.57%	9.633%
85	12.421	1857	1859	1861	rBV2	2883	2818	0.53%	0.061%
86	12.628	1891	1893	1897	rVB5	2078	2589	0.48%	0.056%
87	12.683	1898	1902	1906	rBV7	7081	9841	1.84%	0.212%
88	12.817	1920	1924	1930	rVB6	11462	18079	3.38%	0.390%
89	12.981	1948	1951	1958	rVB4	10282	14950	2.80%	0.323%
90	13.049	1958	1962	1966	rBV3	5689	9229	1.73%	0.199%
91	13.091	1966	1969	1974	rVB5	2878	4872	0.91%	0.105%
92	13.207	1985	1988	1992	rBV3	5935	6972	1.31%	0.150%
93	13.292	1999	2002	2008	rVB2	9929	13805	2.58%	0.298%
94	13.414	2019	2022	2025	rBV3	9566	13514	2.53%	0.292%
95	13.701	2066	2069	2072	rBV4	5392	6740	1.26%	0.145%
96	13.798	2082	2085	2089	rBV4	9542	11436	2.14%	0.247%
97	13.841	2089	2092	2096	rBV	12902	16791	3.14%	0.362%
98	14.615	2215	2219	2225	rBV2	14926	20532	3.84%	0.443%
99	15.213	2314	2317	2321	rVB2	18290	20843	3.90%	0.450%
100	15.420	2347	2351	2356	rVB	22837	32731	6.13%	0.706%

Sum of corrected areas: 4634636

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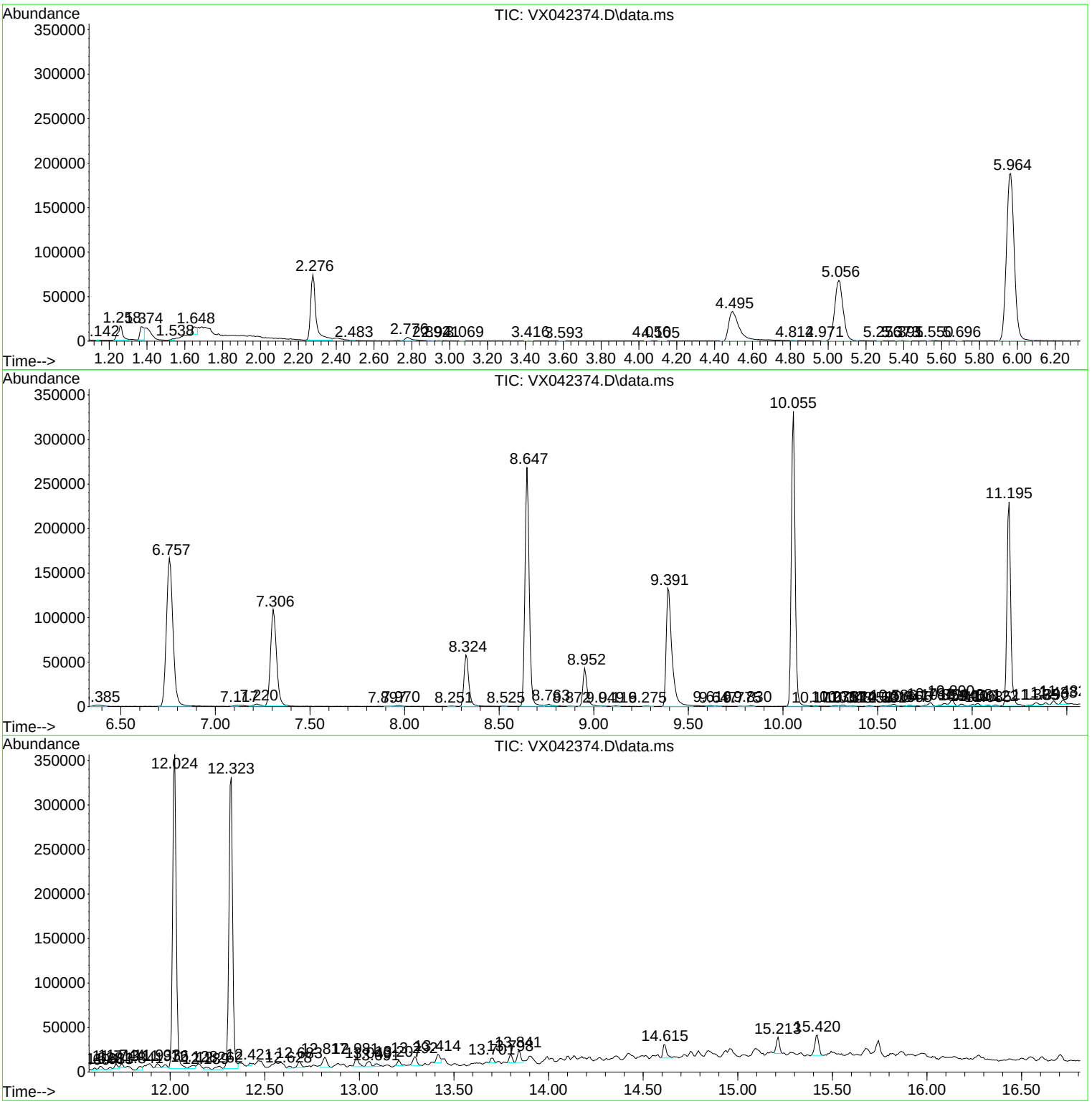
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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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Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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

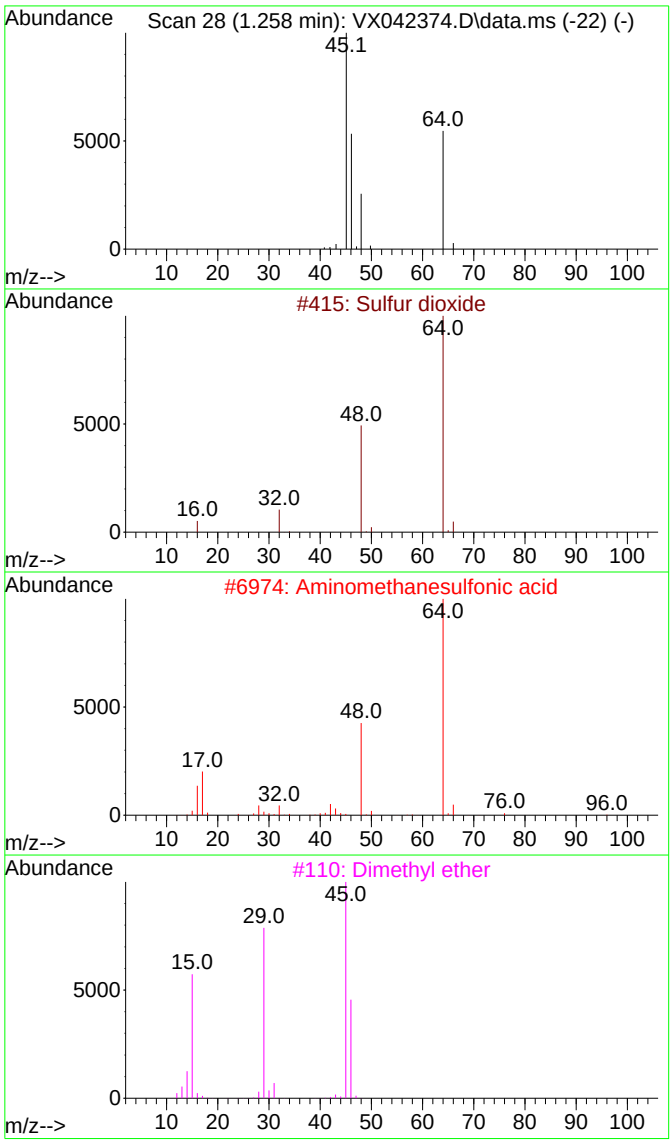
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

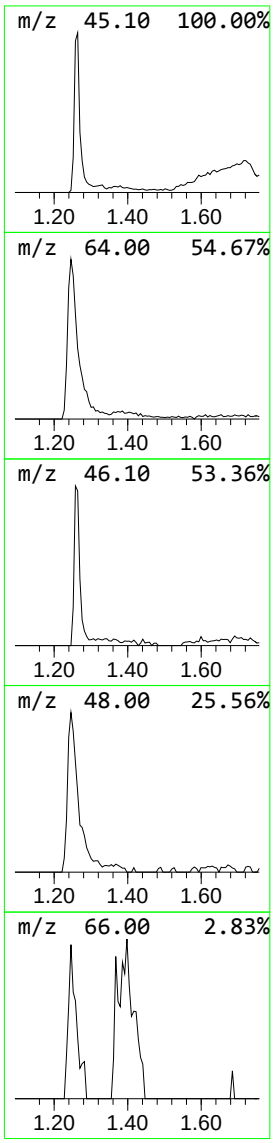
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	3.68 ug/L	29303	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	38
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	38
3	Dimethyl ether	46	C2H6O	000115-10-6	16
4	Dimethyl ether	46	C2H6O	000115-10-6	9
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D24ME

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

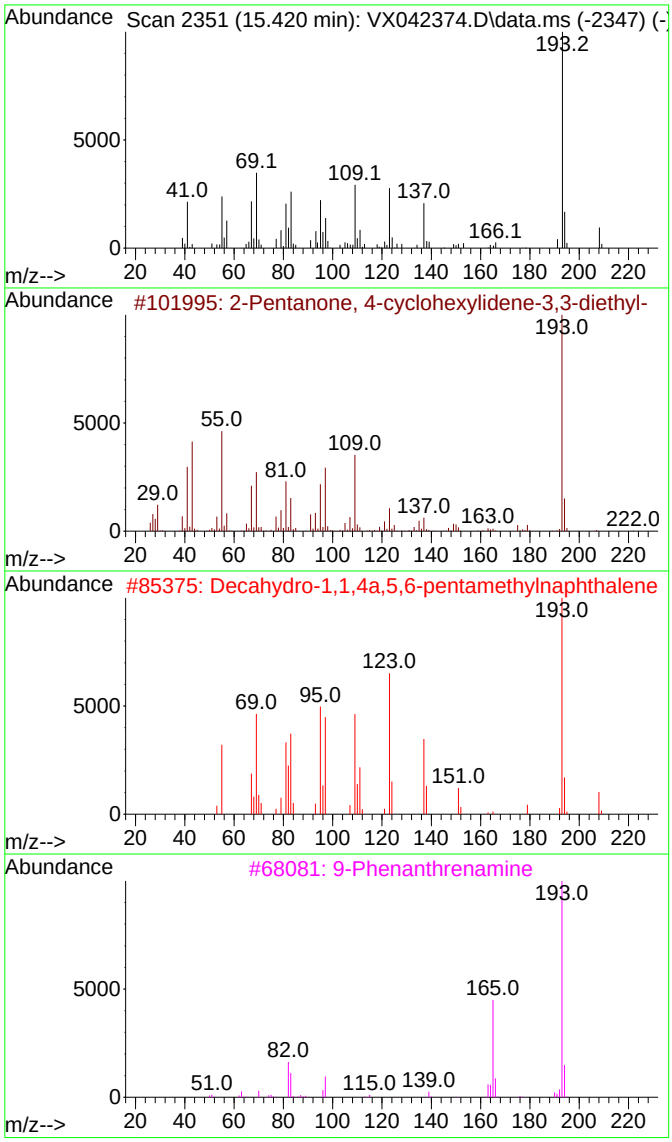
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

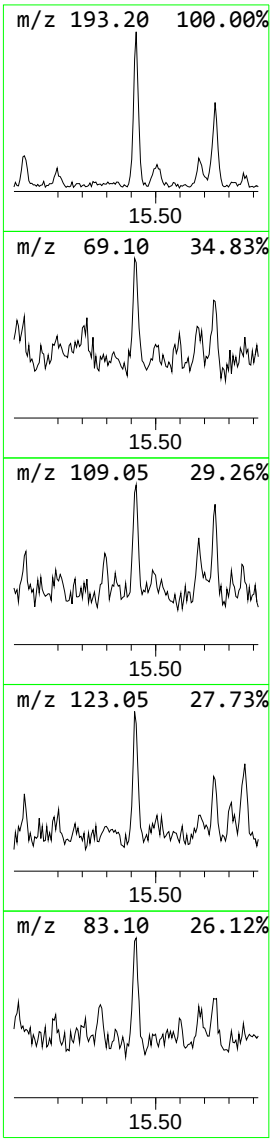
****

Peak Number 3 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.420	3.53 ug/L	32731	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38
3	9-Phenanthrenamine	193	C14H11N	000947-73-9	35
4	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	32
5	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	30





Tentatively Identified Compound (LSC) summary

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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	3.7	ug/L	29303	1	6.757	397684	50.0
unknown-02	15.420	3.5	ug/L	32731	3	12.024	463472	50.0