LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44L9DL

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_U\Method\SFAMULM020823WMA.M
Title : VOC Analysis

Signal : TIC: VU053006.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	44	52	67	rVB	239277	312853	14.65%	2.550%
2	1.534	122	138	141	rBV	15756	39876	1.87%	0.325%
3	1.598	151	158	172	rVB	187353	219848	10.30%	1.792%
4	1.913	250	256	276	rVB	154020	211860	9.92%	1.727%
5	2.566	448	459	475	rVB	290523	478145	22.40%	3.897%
6	2.962	579	582	583	rBV3	1330	789	0.04%	0.006%
7	3.023	598	601	603	rBV3	1778	1350	0.06%	0.011%
8	3.097	621	624	627	rBV5	1138	815	0.04%	0.007%
9	3.180	637	650	661	rBV2	6544	14916	0.70%	0.122%
10	3.280	676	681	685	rBV5	1813	1941	0.09%	0.016%
11	3.521	754	756	760	rBV4	939	851	0.04%	0.007%
12	3.618	782	786	792	rBV7	1657	1677	0.08%	0.014%
13	3.643	792	794	798	rVB4	1102	745	0.03%	0.006%
14	3.672	800	803	808	rBV6	1161	1208	0.06%	0.010%
15	3.827	848	851	855	rBV5	1132	931	0.04%	0.008%
16	3.888	864	870	872	rBV5	1390	1550	0.07%	0.013%
17	3.933	879	884	887	rVB6	1429	1419	0.07%	0.012%
18	4.048	916	920	923	rBV6	1451	1216	0.06%	0.010%
19	4.074	924	928	932	rVB6	1047	936	0.04%	0.008%
20	4.119	936	942	945	rBV9	1048	985	0.05%	0.008%
21	4.138	945	948	950	rBV4	1064	747	0.03%	0.006%
22	4.251	980	983	985	rBV4	1475	1145	0.05%	0.009%
23	4.335	1005	1009	1013	rBV8	1301	1170	0.05%	0.010%
24	4.441	1039	1042	1045	rBV3	1236	1016	0.05%	0.008%
25	4.476	1049	1053	1055	rBV4	1419	1108	0.05%	0.009%
26	4.627	1085	1100	1104	rBV	85300	170426	7.98%	1.389%
27	4.775	1143	1146	1153	rVB8	1629	1644	0.08%	0.013%
28	4.913	1186	1189	1192	rVB4	1561	1003	0.05%	0.008%
29	4.949	1196	1200	1205	rBV8	770	898	0.04%	0.007%
30	4.974	1205	1208	1212	rBV5	1153	777	0.04%	0.006%
31	5.058	1218	1234	1255	rVB	251243	550041	25.77%	4.483%
32	5.277	1299	1302	1303	rBV3	1574	893	0.04%	0.007%
33	5.405	1340	1342	1346	rVB4	1651	808	0.04%	0.007%
34	5.447	1350	1355	1358	rBV6	1170	961	0.05%	0.008%
35	5.470	1358	1362	1366	rVB6	1119	1156	0.05%	0.009%
36	5.534	1378	1382	1387	rVB7	1446	1165	0.05%	0.009%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A44L9DL

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_U\Method\SFAMULM020823WMA.M
Title : VOC Analysis

37	5.582	1392	1397	1400	rBV7	1508	1485	0.07%	0.012%
38	5.601	1400	1403	1406	rVB5	1927	1357	0.06%	0.011%
39	5.627	1406	1411	1413	rBV6	735	737	0.03%	0.006%
40	5.720	1419	1440	1459	rBV2	495168	1327653	62.19%	10.820%
41	6.010	1525	1530	1531	rBV4	1138	772	0.04%	0.006%
42	6.074	1546	1550	1554	rVB6	1335	989	0.05%	0.008%
43	6.122	1562	1565	1573	rVB10	1764	1926	0.09%	0.016%
44	6.244	1588	1603	1625	rBV	394076	741926	34.75%	6.047%
45	6.402	1650	1652	1656	rVB4	1324	853	0.04%	0.007%
46	6.425	1656	1659	1662	rVB5	1981	969	0.05%	0.008%
47	6.444	1662	1665	1666	rBV3	1228	758	0.04%	0.006%
48	6.540	1683	1695	1705	rBV3	15115	29413	1.38%	0.240%
49	6.685	1727	1740	1760	rVV	304527	590399	27.66%	4.812%
50	6.804	1774	1777	1782	rVB6	2320	2075	0.10%	0.017%
51	6.833	1782	1786	1791	rBV6	1014	1015	0.05%	0.008%
52	7.068	1853	1859	1863	rBV7	1865	1649	0.08%	0.013%
53	7.180	1892	1894	1900	rVB6	1211	1286	0.06%	0.010%
54	7.248	1914	1915	1921	rVB6	1539	1004	0.05%	0.008%
55	7.376	1953	1955	1960	rVB5	1168	878	0.04%	0.007%
56	7.405	1960	1964	1967	rBV6	1023	1082	0.05%	0.009%
57	7.476	1981	1986	1989	rBV8	1180	1089	0.05%	0.009%
58	7.563	2000	2013	2028	rBV	199912	358333	16.79%	2.920%
59	7.894	2103	2116	2132	rBV	664940	1149713	53.86%	9.370%
60	8.174	2192	2203	2224	rBV	141371	238737	11.18%	1.946%
61	8.328	2248	2251	2255	rVB5	1405	899	0.04%	0.007%
62	8.395	2270	2272	2277	rVB6	1204	776	0.04%	0.006%
63	8.550	2315	2320	2321	rBV5	1845	1321	0.06%	0.011%
64	8.630	2332	2345	2371	rBV2	264847	505836	23.69%	4.123%
65	8.772	2384	2389	2392	rVB7	1005	908	0.04%	0.007%
66	8.842	2407	2411	2414	rBV5	858	852	0.04%	0.007%
67	9.412	2576	2588	2619	rVV2	544644	1243853	58.26%	10.137%
68	9.781	2701	2703	2710	rVB8	1829	1436	0.07%	0.012%
69	9.813	2710	2713	2718	rBV7	800	786	0.04%	0.006%
70	9.858	2725	2727	2732	rVB5	1032	761	0.04%	0.006%
71	9.891	2732	2737	2741	rBV6	1337	1455	0.07%	0.012%
72	10.019	2773	2777	2780	rBV6	942	936	0.04%	0.008%
73	10.209	2830	2836	2839	rBV7	1365	1394	0.07%	0.011%
74	10.321	2868	2871	2875	rVB5	1247	750	0.04%	0.006%
75	10.482	2919	2921	2927	rVB7	2221	1986	0.09%	0.016%
76	10.749	2992	3004	3019	rBV	418267	677129	31.72%	5.519%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : A44L9DL

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_U\Method\SFAMULM020823WMA.M
Title : VOC Analysis

77	11.083	3104	3108	3111	rBV5	1550	1295	0.06%	0.011%
78	11.392	3202	3204	3211	rBV7	1656	1672	0.08%	0.014%
79	11.469	3225	3228	3233	rVB6	2429	2109	0.10%	0.017%
80	11.743	3306	3313	3321	rBV2	10558	14931	0.70%	0.122%
81	11.807	3321	3333	3356	rBV2	599808	1092204	51.16%	8.901%
82	12.058	3408	3411	3414	rBV4	1202	922	0.04%	0.008%
83	12.083	3416	3419	3422	rVV5	1140	737	0.03%	0.006%
84	12.119	3427	3430	3432	rBV4	1144	795	0.04%	0.006%
85	12.199	3439	3455	3478	rBV2	879438	2134827	100.00%	17.399%
86	12.498	3541	3548	3550	rBV6	1722	1634	0.08%	0.013%
87	12.987	3697	3700	3702	rBV4	1267	938	0.04%	0.008%
88	13.106	3735	3737	3743	rBV7	1405	1397	0.07%	0.011%
89	13.305	3795	3799	3801	rBV5	1674	1253	0.06%	0.010%
90	13.479	3851	3853	3860	rVB9	1765	1439	0.07%	0.012%
91	13.691	3914	3919	3921	rBV6	1456	1327	0.06%	0.011%
92	13.836	3955	3964	3978	rBV	35563	59486	2.79%	0.485%
93	13.987	4008	4011	4013	rBV5	1306	741	0.03%	0.006%
94	14.087	4038	4042	4053	rVB3	5602	8890	0.42%	0.072%
95	14.328	4112	4117	4125	rVB4	8643	11051	0.52%	0.090%
96	14.472	4159	4162	4165	rBV4	1802	1242	0.06%	0.010%
97	14.733	4238	4243	4245	rBV6	1139	986	0.05%	0.008%
98	14.845	4275	4278	4281	rBV6	1667	1465	0.07%	0.012%
99	15.193	4383	4386	4387	rBV3	2687	1323	0.06%	0.011%
100	15.582	4504	4507	4509	rBV4	1827	1277	0.06%	0.010%

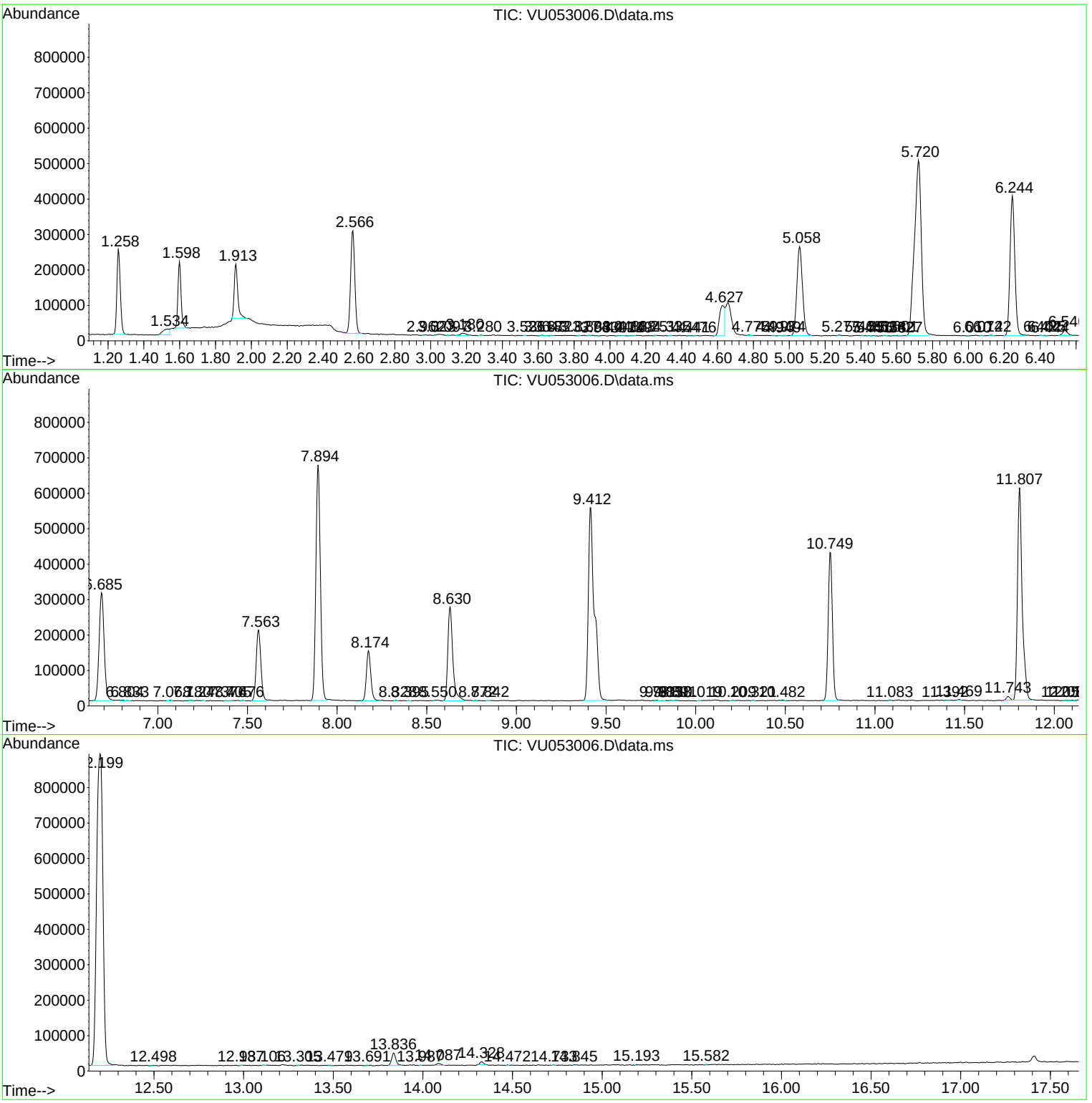
Sum of corrected areas: 12269986

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44L9DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44L9DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

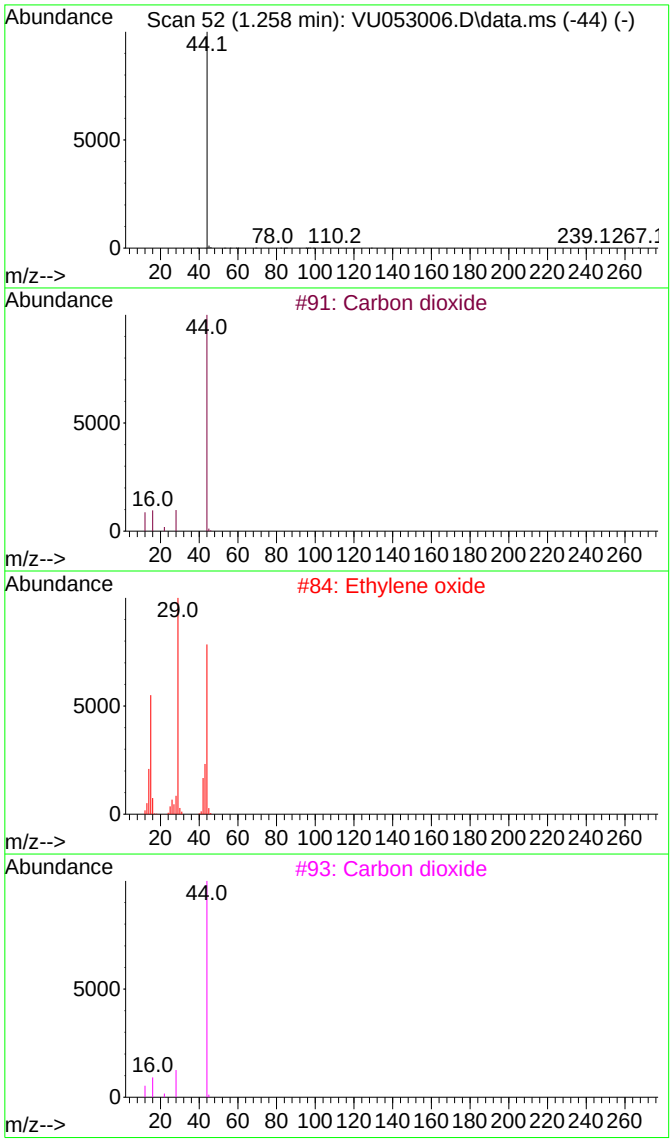
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

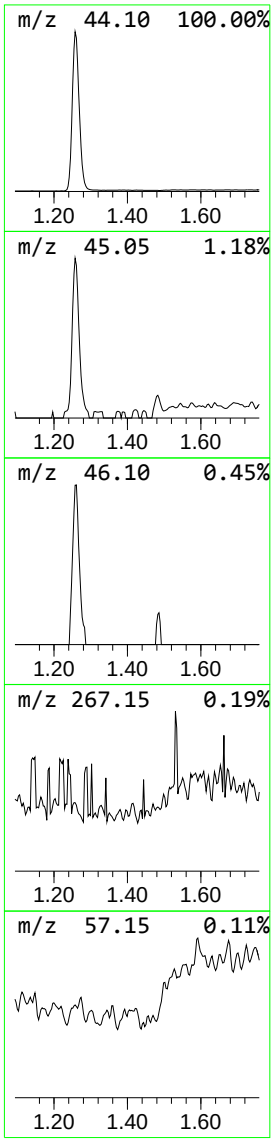
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	21.08 ug/L	312853	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbon dioxide	44	CO2	000124-38-9	4
2	Ethylene oxide	44	C2H4O	000075-21-8	3
3	Carbon dioxide	44	CO2	000124-38-9	3
4	Carbon dioxide	44	CO2	000124-38-9	3
5	Nitrous oxide	44	N2O	010024-97-2	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44L9DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.M
Quant Title : VOC Analysis

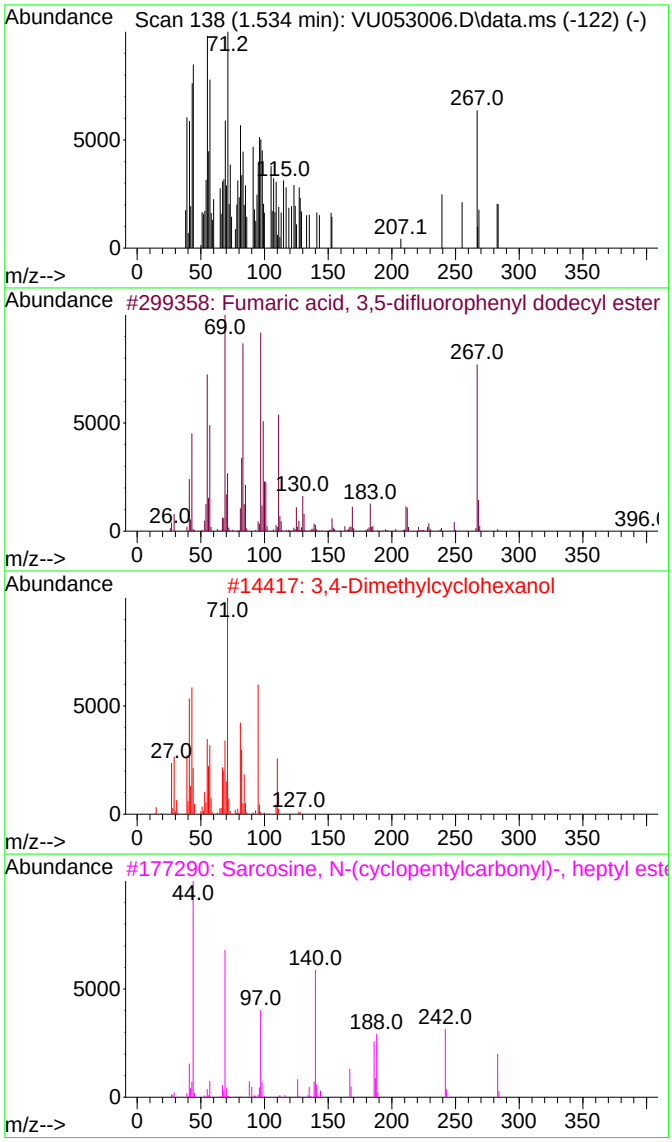
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

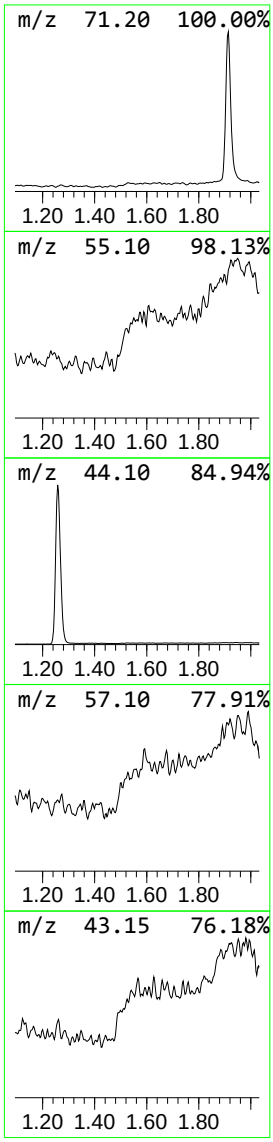
****

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.534	2.69 ug/L	39876	1,4-Difluorobenzene	6.244

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 3,5-difluorophenyl...	396	C22H30F2O4	1000339-37-8	14
2	3,4-Dimethylcyclohexanol	128	C8H16O	005715-23-1	14
3	Sarcosine, N-(cyclopentylcarbony...	283	C16H29NO3	1000321-33-8	14
4	Eicosyl nonyl ether	424	C29H60O	1000406-37-8	14
5	13-Octadecenal, (Z)-	266	C18H34O	058594-45-9	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020823\
Data File : VU053006.D
Acq On : 08 Feb 2023 17:59
Operator : JC/MD
Sample : 01412-02DL 5X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44L9DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020823WMA.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	21.1	ug/L	312853	1	6.244	741926	50.0
unknown-02	1.534	2.7	ug/L	39876	1	6.244	741926	50.0