LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067173.D
Acq On : 26 May 2021 17:42
Operator : JC/MD
Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_N\methods\82N052121W.M
Title : SW846 8260

Signal : TIC: VN067173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.056	114	118	125	rVB8	23613	18486	1.44%	0.197%
2	2.094	125	132	134	rBV8	21022	16541	1.29%	0.176%
3	2.107	134	137	142	rVV6	31979	29806	2.32%	0.318%
4	2.145	142	151	155	rVB10	52183	70303	5.47%	0.750%
5	2.405	240	248	249	rBV6	28938	17425	1.35%	0.186%
6	2.434	255	259	263	rBV6	23826	19577	1.52%	0.209%
7	2.461	263	269	271	rBV6	82992	69095	5.37%	0.737%
8	2.501	281	284	285	rBV2	35580	18567	1.44%	0.198%
9	2.697	354	357	364	rVB8	39213	35619	2.77%	0.380%
10	2.740	364	373	377	rBV8	63296	91191	7.09%	0.973%
11	2.853	409	415	419	rBV8	26662	33835	2.63%	0.361%
12	2.906	431	435	438	rBV5	42452	24456	1.90%	0.261%
13	3.027	468	480	486	rBV5	73529	141473	11.00%	1.509%
14	3.051	486	489	498	rVB10	65495	55092	4.28%	0.588%
15	3.121	511	515	523	rVB8	24183	17914	1.39%	0.191%
16	3.158	524	529	531	rBV4	40994	31062	2.41%	0.331%
17	3.174	531	535	539	rBV6	31722	28187	2.19%	0.301%
18	3.300	576	582	586	rBV9	36746	37505	2.92%	0.400%
19	3.362	601	605	608	rBV6	19494	14247	1.11%	0.152%
20	3.416	621	625	632	rBV9	23520	23347	1.82%	0.249%
21	3.456	636	640	644	rVB6	47592	33363	2.59%	0.356%
22	3.477	644	648	652	rBV6	25254	29810	2.32%	0.318%
23	3.544	669	673	677	rVV6	14892	14396	1.12%	0.154%
24	3.566	677	681	686	rVB8	27476	27968	2.17%	0.298%
25	3.735	738	744	745	rBV6	29627	20687	1.61%	0.221%
26	3.748	745	749	753	rVB6	37022	31814	2.47%	0.339%
27	3.826	768	778	782	rBV6	29674	49607	3.86%	0.529%
28	3.909	806	809	812	rBV4	16823	15177	1.18%	0.162%
29	3.925	812	815	823	rVB8	49222	46605	3.62%	0.497%
30	4.000	835	843	846	rBV7	25174	21775	1.69%	0.232%
31	4.035	851	856	859	rBV7	43457	44958	3.50%	0.480%
32	4.076	866	871	872	rBV5	36618	26198	2.04%	0.280%
33	4.175	902	908	909	rBV6	34913	28780	2.24%	0.307%
34	4.261	936	940	942	rBV4	26625	18401	1.43%	0.196%
35	4.317	956	961	965	rBV7	18625	17718	1.38%	0.189%
36	4.580	1057	1059	1063	rVB4	25084	13034	1.01%	0.139%

LSC Area Percent Report

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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Title : SW846 8260

37	4.722	1109	1112	1118	rBV7	21786	17249	1.34%	0.184%
38	4.773	1126	1131	1136	rBV8	39877	39076	3.04%	0.417%
39	4.802	1137	1142	1147	rVV9	47912	52600	4.09%	0.561%
40	4.824	1147	1150	1155	rVB6	55747	43809	3.41%	0.467%
41	4.851	1155	1160	1163	rBV6	47088	35773	2.78%	0.382%
42	4.875	1163	1169	1177	rVB10	48225	77025	5.99%	0.822%
43	4.936	1188	1192	1194	rBV3	39218	28131	2.19%	0.300%
44	5.119	1251	1260	1266	rBV10	50750	84647	6.58%	0.903%
45	5.242	1301	1306	1310	rBV7	47718	40703	3.16%	0.434%
46	5.266	1310	1315	1318	rBV6	38663	29199	2.27%	0.312%
47	5.282	1318	1321	1324	rBV5	25549	21900	1.70%	0.234%
48	5.366	1345	1352	1356	rBV9	48948	42920	3.34%	0.458%
49	5.430	1369	1376	1379	rBV9	19942	20683	1.61%	0.221%
50	5.449	1379	1383	1389	rVV7	55840	54385	4.23%	0.580%
51	5.484	1392	1396	1402	rVB6	33919	22785	1.77%	0.243%
52	5.543	1409	1418	1423	rBV9	41822	41700	3.24%	0.445%
53	5.594	1430	1437	1439	rVV7	52584	52392	4.07%	0.559%
54	5.610	1439	1443	1452	rVB7	63070	71904	5.59%	0.767%
55	5.655	1458	1460	1463	rVB4	45646	23286	1.81%	0.248%
56	5.800	1510	1514	1517	rVV5	41131	32516	2.53%	0.347%
57	5.824	1521	1523	1526	rVV4	34701	19928	1.55%	0.213%
58	5.843	1526	1530	1536	rVB6	22014	19627	1.53%	0.209%
59	5.953	1568	1571	1580	rBV10	25728	21280	1.65%	0.227%
60	5.998	1582	1588	1590	rBV6	23729	21841	1.70%	0.233%
61	6.052	1602	1608	1611	rBV7	21425	15635	1.22%	0.167%
62	6.133	1630	1638	1640	rBV8	22123	22714	1.77%	0.242%
63	6.184	1648	1657	1660	rBV7	27302	29493	2.29%	0.315%
64	6.205	1660	1665	1669	rVV8	32397	38215	2.97%	0.408%
65	6.226	1669	1673	1677	rVV6	40688	40228	3.13%	0.429%
66	6.251	1680	1682	1689	rVB7	24345	19508	1.52%	0.208%
67	6.304	1697	1702	1703	rBV3	60506	35445	2.76%	0.378%
68	6.318	1705	1707	1715	rVB7	69975	70970	5.52%	0.757%
69	6.479	1762	1767	1773	rBV8	36713	50370	3.92%	0.537%
70	6.511	1775	1779	1783	rVV6	43933	41285	3.21%	0.440%
71	6.731	1855	1861	1867	rBV8	45111	46635	3.63%	0.498%
72	6.752	1867	1869	1874	rVB6	24841	19989	1.55%	0.213%
73	7.122	2001	2007	2013	rBV8	33286	33937	2.64%	0.362%
74	7.216	2036	2042	2050	rVB8	49954	43999	3.42%	0.469%
75	7.377	2097	2102	2108	rVB4	76660	49402	3.84%	0.527%
76	7.516	2131	2154	2168	rBV2	156056	399053	31.02%	4.258%

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Instrument : MSVOA_N
ClientSampleId : 31046

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77	7.597	2168	2184	2207	rVB2	270748	677289	52.66%	7.226%
78	7.959	2295	2319	2349	rBV2	188511	467393	36.34%	4.987%
79	8.522	2511	2529	2572	rBV	442459	976310	75.90%	10.417%
80	9.397	2850	2855	2860	rVB8	18864	13547	1.05%	0.145%
81	10.038	3076	3094	3139	rBV	667163	1286235	100.00%	13.723%
82	11.360	3566	3587	3635	rBV	525852	1082413	84.15%	11.549%
83	12.357	3942	3959	4011	rBV2	285689	738217	57.39%	7.876%
84	13.302	4296	4311	4341	rBV	338332	838610	65.20%	8.947%
85	13.444	4361	4364	4371	rVB6	33794	17078	1.33%	0.182%
86	15.219	5023	5026	5032	rBV7	19300	15525	1.21%	0.166%
87	16.525	5509	5513	5516	rBV6	19416	17513	1.36%	0.187%
88	16.552	5518	5523	5529	rVB8	38621	34781	2.70%	0.371%
89	16.584	5530	5535	5538	rBV4	51503	48993	3.81%	0.523%
90	16.638	5550	5555	5562	rVB9	33342	34661	2.69%	0.370%
91	16.785	5603	5610	5614	rBV10	14896	17812	1.38%	0.190%

Sum of corrected areas: 9372633

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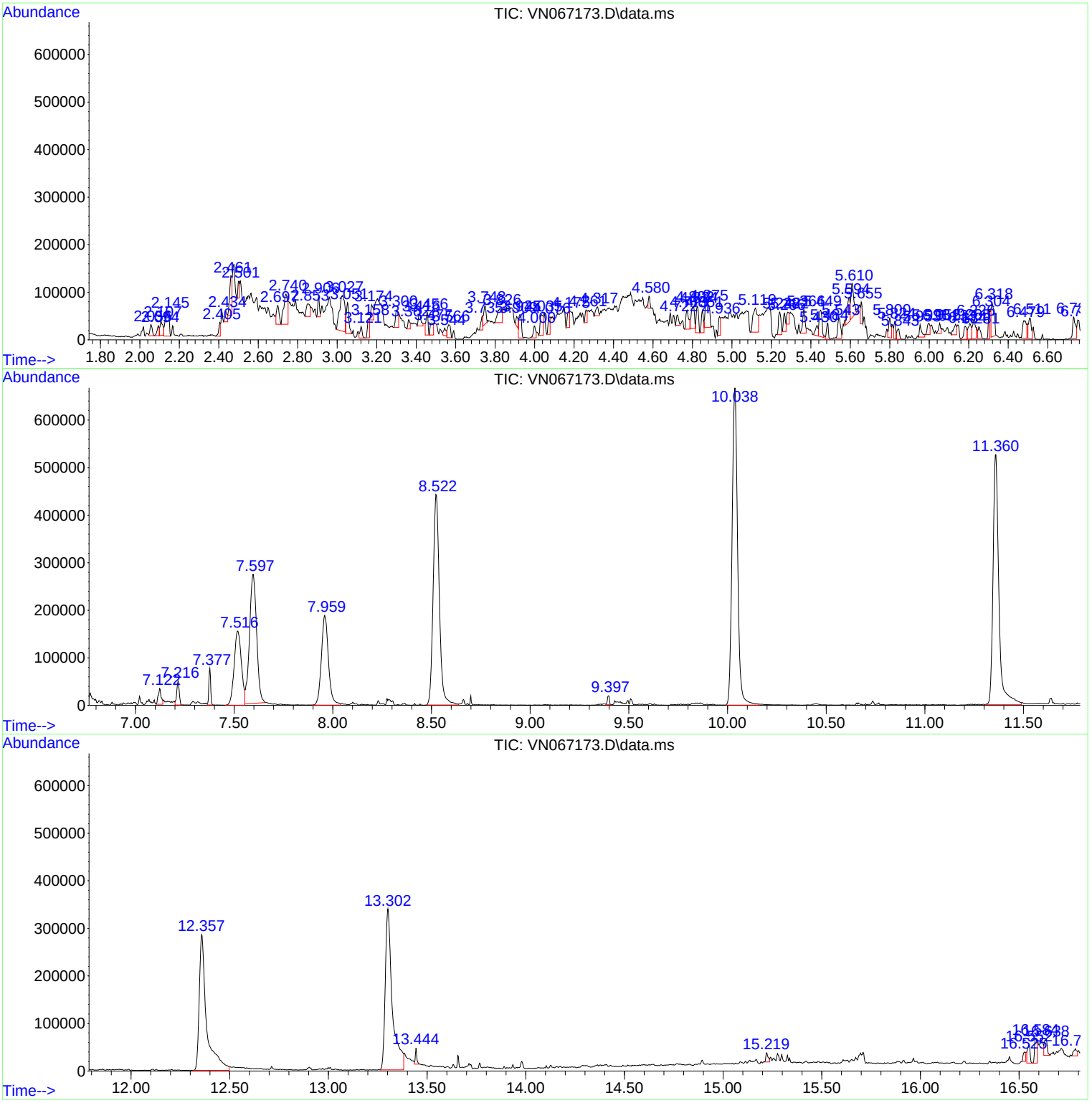
MSVOA_N
ClientSampleId :
31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
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Acq On : 26 May 2021 17:42
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

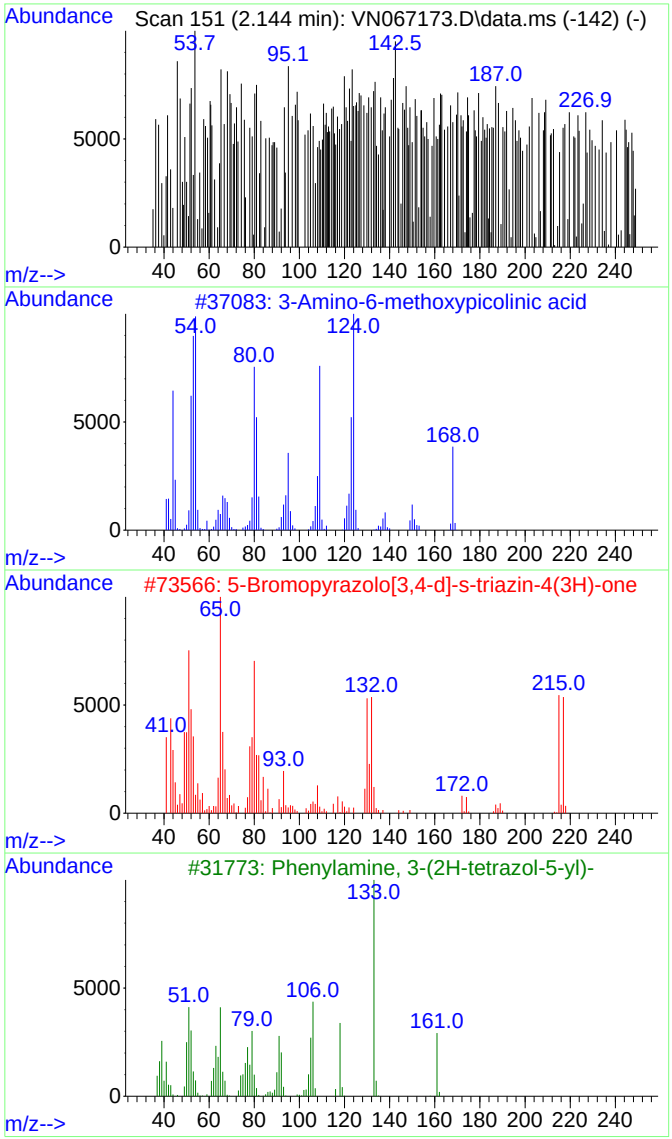
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

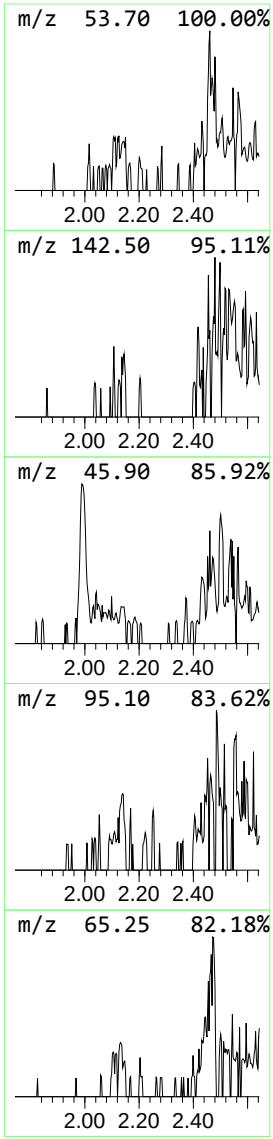
****

Peak Number 1 unknown2.144 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.144	5.19 ug/l	70303	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Amino-6-methoxypicolinic acid	168	C7H8N2O3	1000214-53-7	43
2	5-Bromopyrazolo[3,4-d]-s-triazin...	215	C4H2BrN5O	1000212-45-5	41
3	Phenylamine, 3-(2H-tetrazol-5-yl)-	161	C7H7N5	1000315-93-5	35
4	2-Pyridinemethanamine	108	C6H8N2	003731-51-9	35
5	Acetamide, 2-(hydroxyimino)-N-(2...	178	C9H10N2O2	001132-03-2	35





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Operator : JC/MD
Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

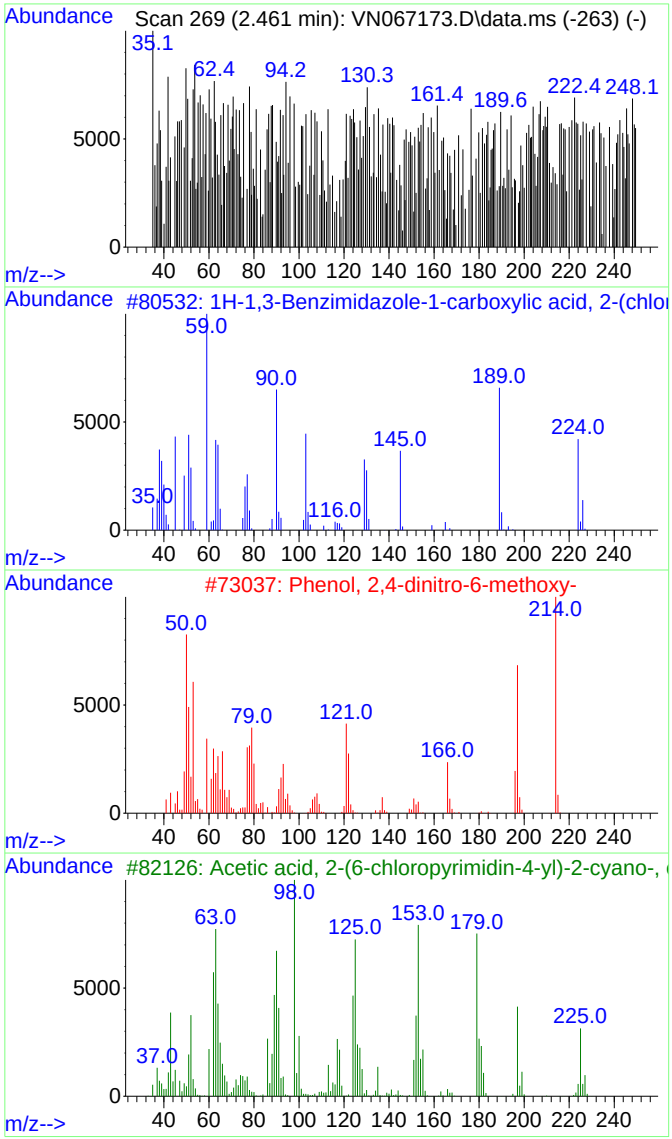
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

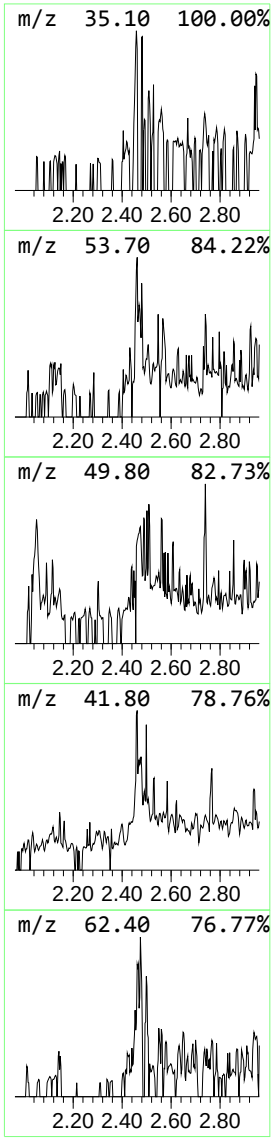
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-1,3-Benzimidazole-1-carb... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.461	5.10 ug/l	69095	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,3-Benzimidazole-1-carboxyli...	224	C10H9ClN2O2	1000362-72-3	55
2	Phenol, 2,4-dinitro-6-methoxy-	214	C7H6N2O6	004097-63-6	46
3	Acetic acid, 2-(6-chloropyrimidi...	225	C9H8ClN3O2	1000264-26-9	46
4	Benzenecarboximidoyl chloride, N...	185	C8H8ClNO2	1000362-64-9	41
5	Ambrosin	246	C15H18O3	000509-93-3	41





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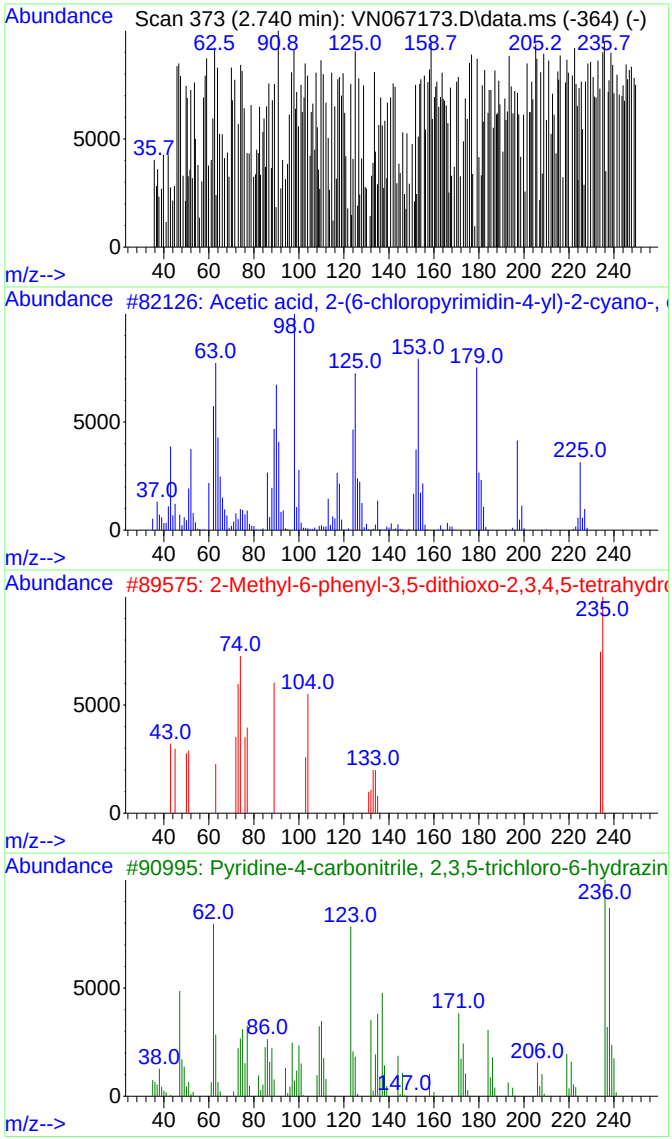
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

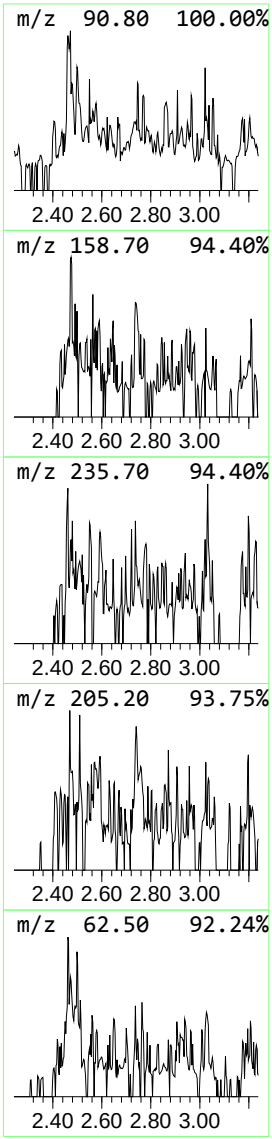
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Acetic acid, 2-(6-chloropyr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.740	6.73 ug/l	91191	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-(6-chloropyrimidi...	225	C9H8ClN3O2	1000264-26-9	60
2	2-Methyl-6-phenyl-3,5-dithioxo-2...	235	C10H9N3S2	038119-56-1	53
3	Pyridine-4-carbonitrile, 2,3,5-t...	236	C6H3Cl3N4	085228-63-3	44
4	6-Nitropiperonal	195	C8H5NO5	000712-97-0	44
5	4-Hydroxy-2-methoxybenzaldehyde,...	224	C11H16O3Si	1000352-91-5	41





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Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
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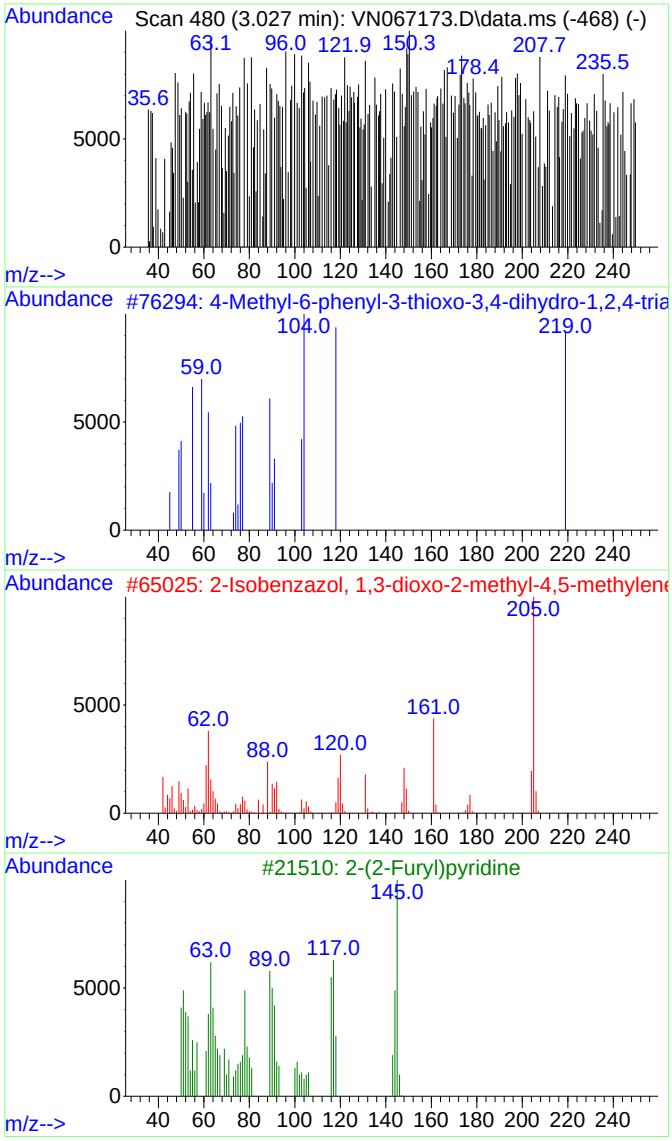
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

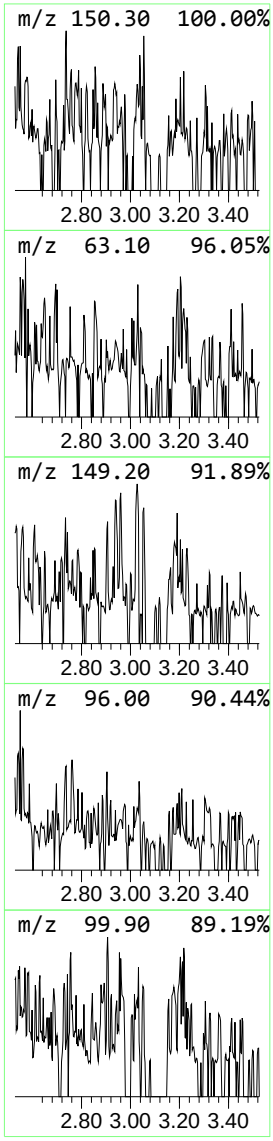
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Methyl-6-phenyl-3-thioxo-... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.027	10.44 ug/l	141473	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methyl-6-phenyl-3-thioxo-3,4-d...	219	C10H9N3OS	022936-87-4	92
2	2-Isobenzazol, 1,3-dioxo-2-methy...	205	C10H7NO4	1000111-66-6	87
3	2-(2-Furyl)pyridine	145	C9H7NO	055484-03-2	87
4	Benzeneacetic acid, 2-carboxy-3-...	210	C10H10O5	001137-31-1	83
5	4H-1-Benzopyran-4-one, 6-bromo-	224	C9H5BrO2	051483-92-2	53





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Instrument : MSVOA_N
ClientSampleId : 31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

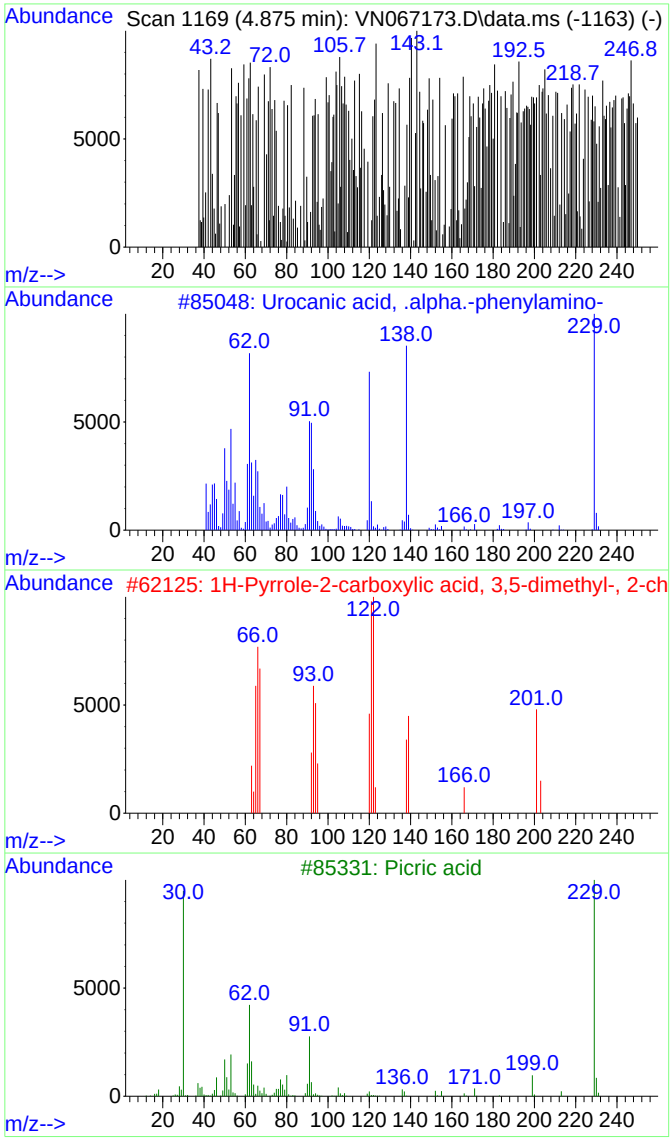
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

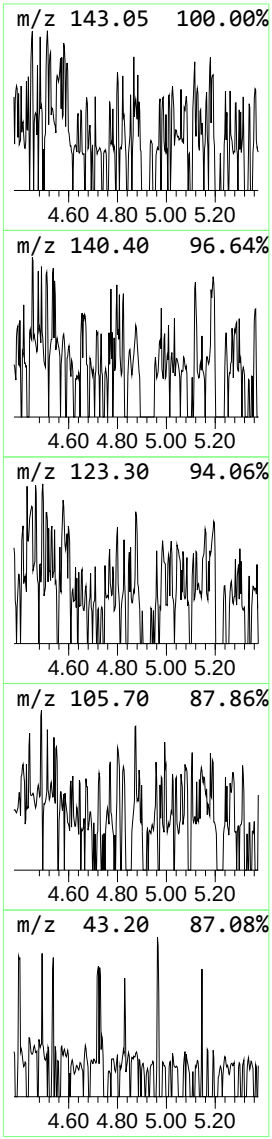
****

Peak Number 5 unknown4.875 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	5.69 ug/l	77025	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urocanic acid, .alpha.-phenylamino-	229	C12H11N3O2	1000128-69-4	42
2	1H-Pyrrole-2-carboxylic acid, 3,...	201	C9H12ClNO2	035889-92-0	38
3	Picric acid	229	C6H3N3O7	000088-89-1	25
4	Ethanone, 1-(2-furanyl)-, [1-(2-...	216	C12H12N2O2	024523-53-3	25
5	Oxazole, 4-benzyl-5-methyl-	173	C11H11NO	103987-33-3	25





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Instrument : MSVOA_N
ClientSampleId : 31046

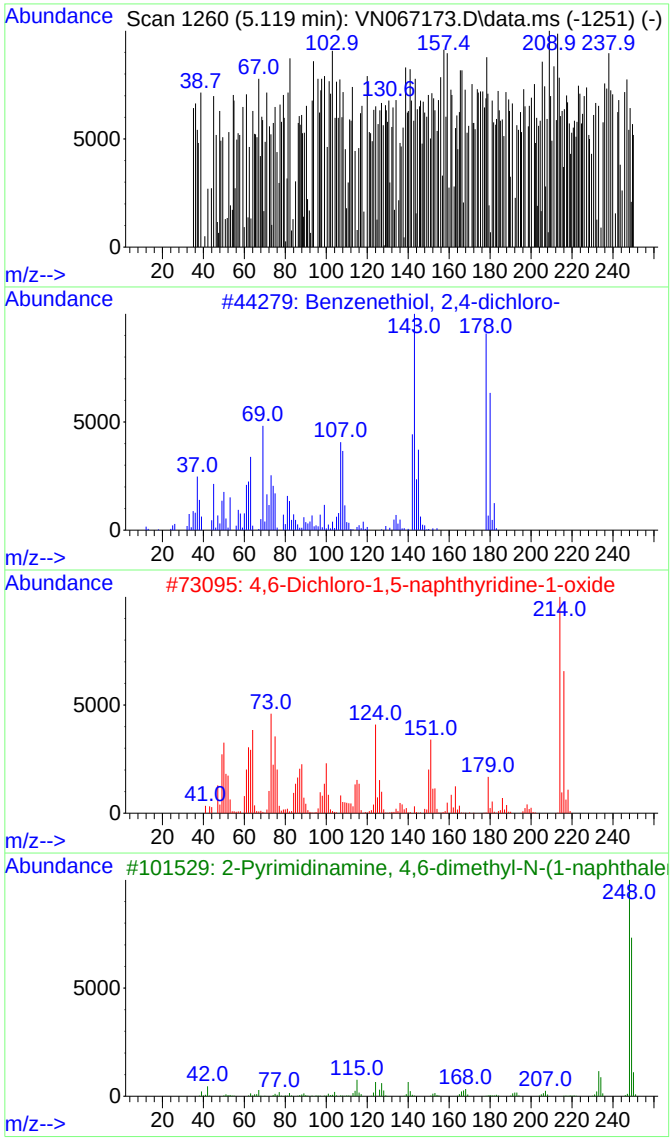
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

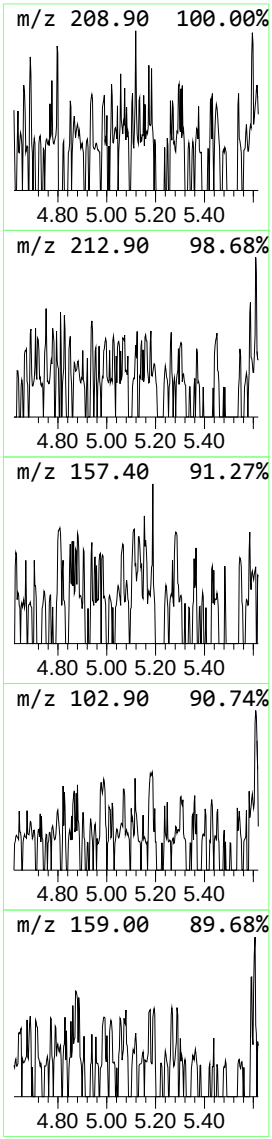
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzenethiol, 2,4-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.119	6.25 ug/l	84647	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 2,4-dichloro-	178	C6H4Cl2S	001122-41-4	83
2	4,6-Dichloro-1,5-naphthyridine-1...	214	C8H4Cl2N2O	1000213-90-4	56
3	2-Pyrimidinamine, 4,6-dimethyl-N...	249	C16H15N3	1000317-28-2	45
4	5-Bromopyrazolo[3,4-d]-s-triazin...	215	C4H2BrN5O	1000212-45-5	44
5	1,3,4-Oxadiazole, 2-(chloromethy...	238	C11H11ClN2O2	1000337-10-6	41





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067173.D
Acq On : 26 May 2021 17:42
Operator : JC/MD
Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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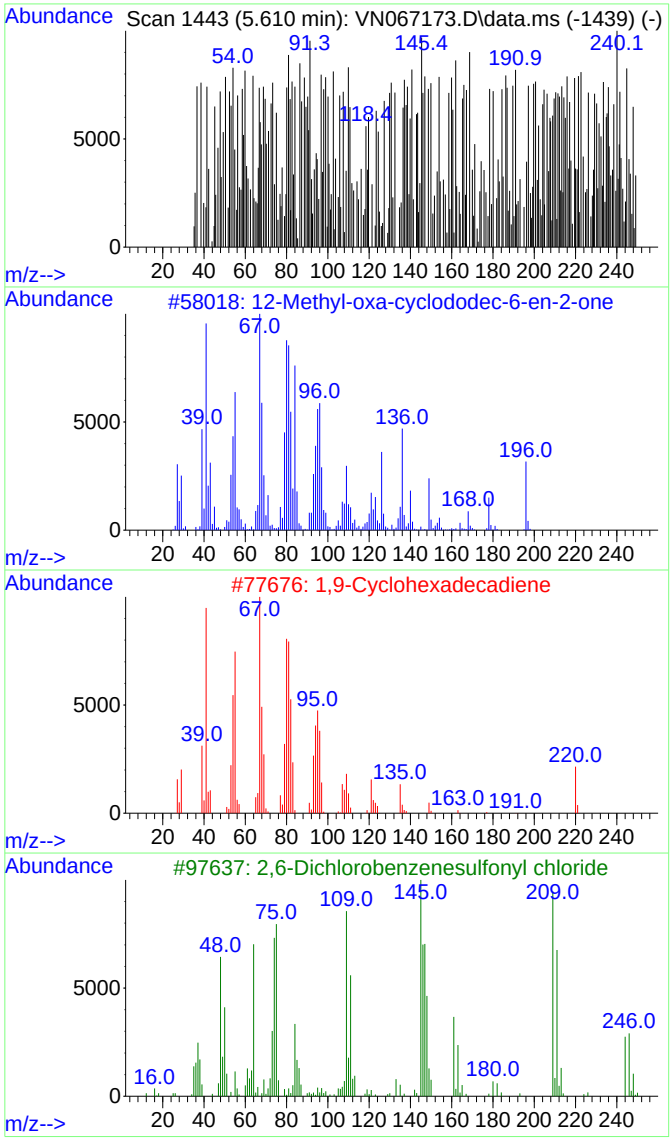
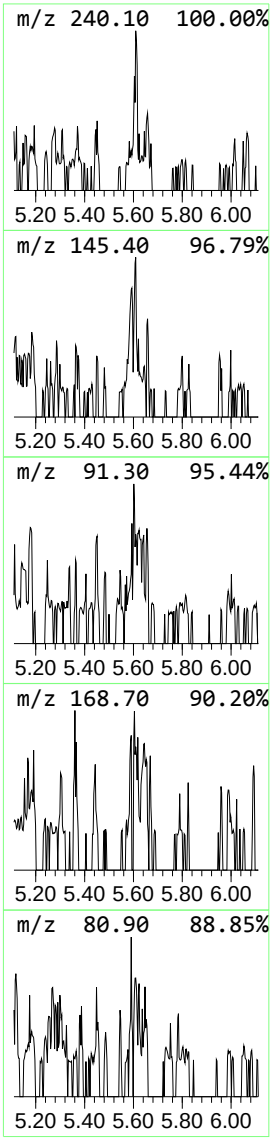
Peak Number 7 unknown5.610 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.610	5.31 ug/l	71904	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Methyl-oxa-cyclododec-6-en-2-one	196	C12H20O2	1000194-34-2	43
2	1,9-Cyclohexadecadiene	220	C16H28	004277-06-9	40
3	2,6-Dichlorobenzenesulfonyl chlo...	244	C6H3Cl3O2S	006579-54-0	38
4	1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	25
5	1,2,5-Triazole, 1-(3-propenyl)-3...	213	C6H7N5O4	311314-76-8	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067173.D
Acq On : 26 May 2021 17:42
Operator : JC/MD
Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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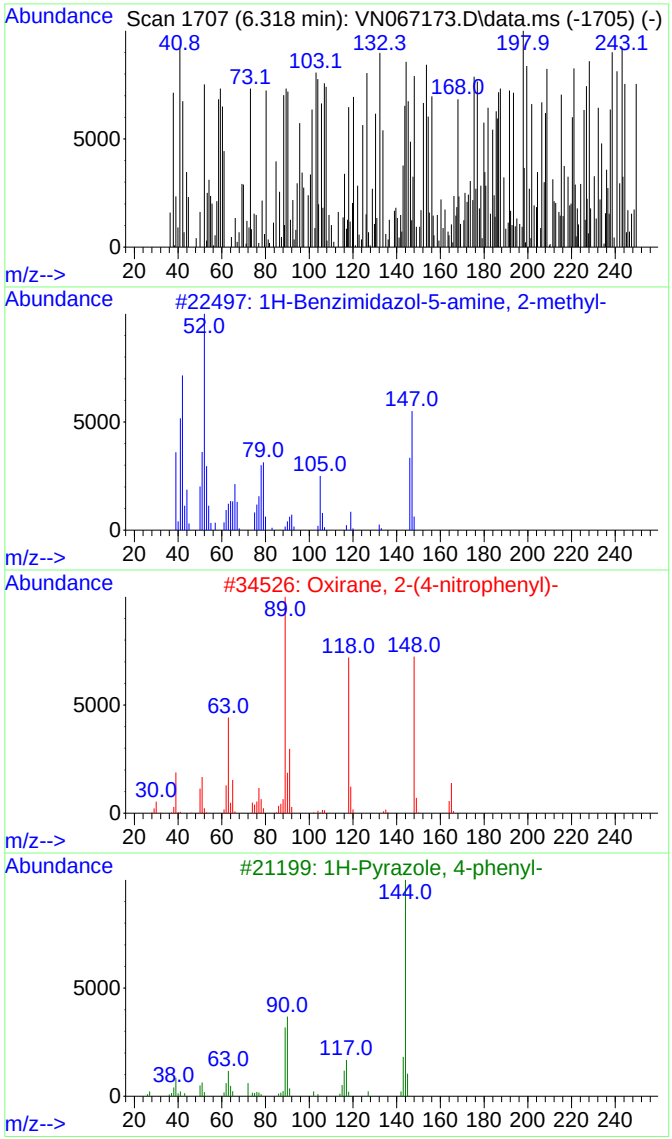
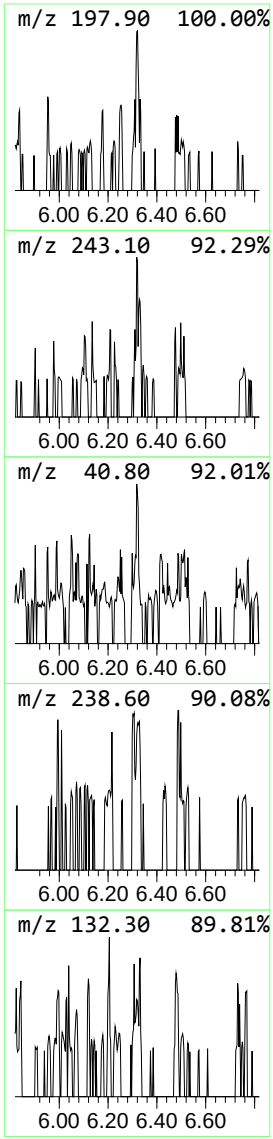
Peak Number 8 unknown6.318 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.318	5.24 ug/l	70970	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazol-5-amine, 2-methyl-	147	C8H9N3	029043-48-9	25
2	Oxirane, 2-(4-nitrophenyl)-	165	C8H7NO3	1000362-15-5	25
3	1H-Pyrazole, 4-phenyl-	144	C9H8N2	010199-68-5	15
4	1H-Imidazole, 2,4-diphenyl-	220	C15H12N2	000670-83-7	14
5	2-Amino-4-(4-nitrophenyl)thiazole	221	C9H7N3O2S	002104-09-8	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067173.D
Acq On : 26 May 2021 17:42
Operator : JC/MD
Sample : M2529-01 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 31046

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.144	2.144	5.2	ug/l	70303	1	7.597	677289	50.0
1H-1,3-Benzimid...	2.461	5.1	ug/l	69095	1	7.597	677289	50.0
Acetic acid, 2-...	2.740	6.7	ug/l	91191	1	7.597	677289	50.0
4-Methyl-6-phen...	3.027	10.4	ug/l	141473	1	7.597	677289	50.0
unknown4.875	4.875	5.7	ug/l	77025	1	7.597	677289	50.0
Benzenethiol, 2...	5.119	6.3	ug/l	84647	1	7.597	677289	50.0
unknown5.610	5.610	5.3	ug/l	71904	1	7.597	677289	50.0
unknown6.318	6.318	5.2	ug/l	70970	1	7.597	677289	50.0