LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067174.D
Acq On : 26 May 2021 18:05
Operator : JC/MD
Sample : M2529-02 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41791

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: VN067174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.852	36	42	45	rBV5	17565	14993	1.12%	0.152%
2	1.879	45	52	54	rBV7	41094	38599	2.87%	0.393%
3	1.994	88	95	97	rBV7	22313	15824	1.18%	0.161%
4	2.021	101	105	107	rBV4	24631	16184	1.20%	0.165%
5	2.319	206	216	218	rBV8	36662	33597	2.50%	0.342%
6	2.413	247	251	254	rBV5	26845	21276	1.58%	0.216%
7	2.456	258	267	274	rBV10	157698	269571	20.06%	2.741%
8	2.563	302	307	310	rBV7	51305	49252	3.66%	0.501%
9	2.922	438	441	445	rBV5	23651	20890	1.55%	0.212%
10	3.107	506	510	513	rBV6	23408	19852	1.48%	0.202%
11	3.327	586	592	593	rBV6	23672	22089	1.64%	0.225%
12	3.480	646	649	658	rVB10	34582	30954	2.30%	0.315%
13	3.531	661	668	670	rBV7	17482	17546	1.31%	0.178%
14	3.614	695	699	704	rBV6	41402	23259	1.73%	0.237%
15	4.183	906	911	915	rBV5	39816	21460	1.60%	0.218%
16	4.287	944	950	953	rBV6	48537	39493	2.94%	0.402%
17	4.314	957	960	965	rVB6	53608	29597	2.20%	0.301%
18	4.684	1094	1098	1102	rVB3	50287	27250	2.03%	0.277%
19	4.829	1145	1152	1155	rBV5	42914	28673	2.13%	0.292%
20	4.848	1155	1159	1167	rVB8	63116	51072	3.80%	0.519%
21	4.893	1169	1176	1180	rBV7	92051	88508	6.59%	0.900%
22	4.923	1180	1187	1193	rVV10	103599	135817	10.10%	1.381%
23	4.947	1193	1196	1198	rVV3	43696	21137	1.57%	0.215%
24	4.961	1198	1201	1206	rVB4	59087	35004	2.60%	0.356%
25	5.631	1445	1451	1456	rBV8	66916	91047	6.77%	0.926%
26	5.717	1475	1483	1486	rBV9	39184	37808	2.81%	0.384%
27	5.733	1486	1489	1495	rVB7	49761	33093	2.46%	0.337%
28	5.765	1495	1501	1505	rBV7	50605	50519	3.76%	0.514%
29	5.792	1505	1511	1516	rVB7	60214	58241	4.33%	0.592%
30	5.982	1576	1582	1585	rBV6	66718	60265	4.48%	0.613%
31	6.248	1678	1681	1688	rVB4	81980	52089	3.88%	0.530%
32	6.690	1840	1846	1850	rBV6	28363	25538	1.90%	0.260%
33	6.972	1937	1951	1955	rBV6	141539	254332	18.92%	2.586%
34	6.993	1957	1959	1963	rVB4	125759	72516	5.40%	0.737%
35	7.015	1963	1967	1968	rBV2	43701	26805	1.99%	0.273%
36	7.203	2030	2037	2040	rBV5	59238	60367	4.49%	0.614%

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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41791

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Title : SW846 8260

37	7.522	2141	2156	2170	rVV2	145508	391775	29.15%	3.984%
38	7.597	2170	2184	2201	rVB2	269864	640077	47.62%	6.509%
39	7.897	2281	2296	2303	rVB2	37074	60980	4.54%	0.620%
40	7.959	2303	2319	2337	rBV	201871	481933	35.86%	4.901%
41	8.418	2483	2490	2493	rBV8	16481	16986	1.26%	0.173%
42	8.522	2510	2529	2551	rBV	450654	983029	73.14%	9.996%
43	8.764	2613	2619	2626	rVB10	30184	45140	3.36%	0.459%
44	8.836	2642	2646	2650	rVB2	57720	24712	1.84%	0.251%
45	8.887	2656	2665	2669	rBV8	67351	78661	5.85%	0.800%
46	8.943	2682	2686	2688	rBV4	28439	18724	1.39%	0.190%
47	9.067	2725	2732	2738	rVB9	62682	83366	6.20%	0.848%
48	9.104	2740	2746	2751	rBV7	47196	38311	2.85%	0.390%
49	9.407	2855	2859	2862	rBV4	41599	27970	2.08%	0.284%
50	9.506	2890	2896	2900	rBV6	62136	71946	5.35%	0.732%
51	9.563	2914	2917	2920	rVB4	24693	13905	1.03%	0.141%
52	9.582	2920	2924	2926	rBV5	33798	22649	1.69%	0.230%
53	9.595	2926	2929	2933	rVB5	27148	15604	1.16%	0.159%
54	9.675	2957	2959	2965	rVB7	28489	17794	1.32%	0.181%
55	10.037	3072	3094	3112	rBV	703720	1344085	100.00%	13.668%
56	10.099	3112	3117	3119	rVV5	64346	56544	4.21%	0.575%
57	10.121	3120	3125	3131	rVB7	96754	101192	7.53%	1.029%
58	10.316	3194	3198	3201	rBV4	50628	38662	2.88%	0.393%
59	10.413	3231	3234	3237	rBV4	49128	39157	2.91%	0.398%
60	10.982	3439	3446	3451	rBV9	30229	31524	2.35%	0.321%
61	11.006	3451	3455	3457	rBV5	27236	13921	1.04%	0.142%
62	11.022	3457	3461	3466	rBV7	29890	30223	2.25%	0.307%
63	11.134	3497	3503	3507	rBV7	16669	19865	1.48%	0.202%
64	11.357	3572	3586	3609	rBV	569276	1086357	80.83%	11.047%
65	11.912	3788	3793	3799	rVB6	49219	47570	3.54%	0.484%
66	12.154	3877	3883	3888	rBV9	23086	19475	1.45%	0.198%
67	12.199	3894	3900	3904	rBV6	25604	31717	2.36%	0.323%
68	12.277	3921	3929	3933	rBV6	52375	51546	3.84%	0.524%
69	12.357	3946	3959	3972	rBV2	273711	622666	46.33%	6.332%
70	12.419	3979	3982	3989	rVB4	46535	31608	2.35%	0.321%
71	12.454	3991	3995	3997	rVV4	36908	28678	2.13%	0.292%
72	12.470	3999	4001	4007	rVB6	61465	52516	3.91%	0.534%
73	12.508	4011	4015	4019	rVB6	40368	21403	1.59%	0.218%
74	12.564	4030	4036	4038	rBV6	53223	45746	3.40%	0.465%
75	12.599	4042	4049	4051	rBV8	23118	18459	1.37%	0.188%
76	13.055	4212	4219	4223	rBV9	25576	27590	2.05%	0.281%

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Title : SW846 8260

77	13.301	4296	4311	4326	rBV	358262	796613	59.27%	8.101%
78	13.401	4343	4348	4352	rBV9	26779	24027	1.79%	0.244%
79	13.422	4352	4356	4359	rBV5	28834	24317	1.81%	0.247%
80	13.465	4368	4372	4376	rBV6	38397	35881	2.67%	0.365%
81	13.672	4436	4449	4450	rBV6	49102	77448	5.76%	0.788%
82	13.717	4461	4466	4470	rBV7	35992	40171	2.99%	0.408%
83	14.240	4653	4661	4668	rBV7	35575	35444	2.64%	0.360%
84	14.557	4772	4779	4782	rBV7	23022	25800	1.92%	0.262%
85	14.578	4782	4787	4793	rVB8	18160	19792	1.47%	0.201%
86	14.661	4813	4818	4822	rBV7	25215	24686	1.84%	0.251%
87	14.712	4829	4837	4844	rVB7	15977	24677	1.84%	0.251%
88	15.554	5144	5151	5159	rVB10	12307	16437	1.22%	0.167%

Sum of corrected areas: 9833876

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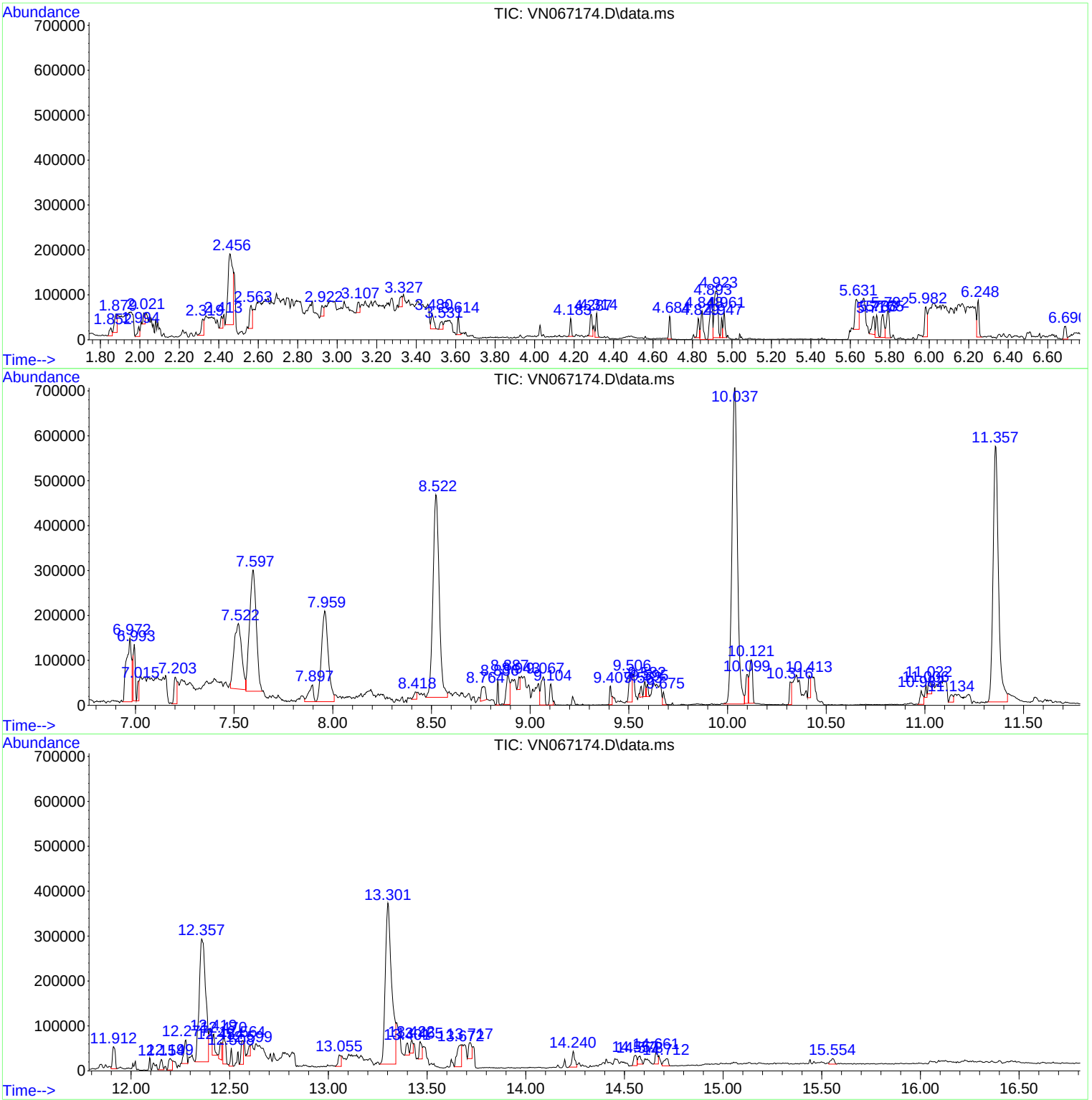
Instrument :
MSVOA_N
ClientSampleId :
41791

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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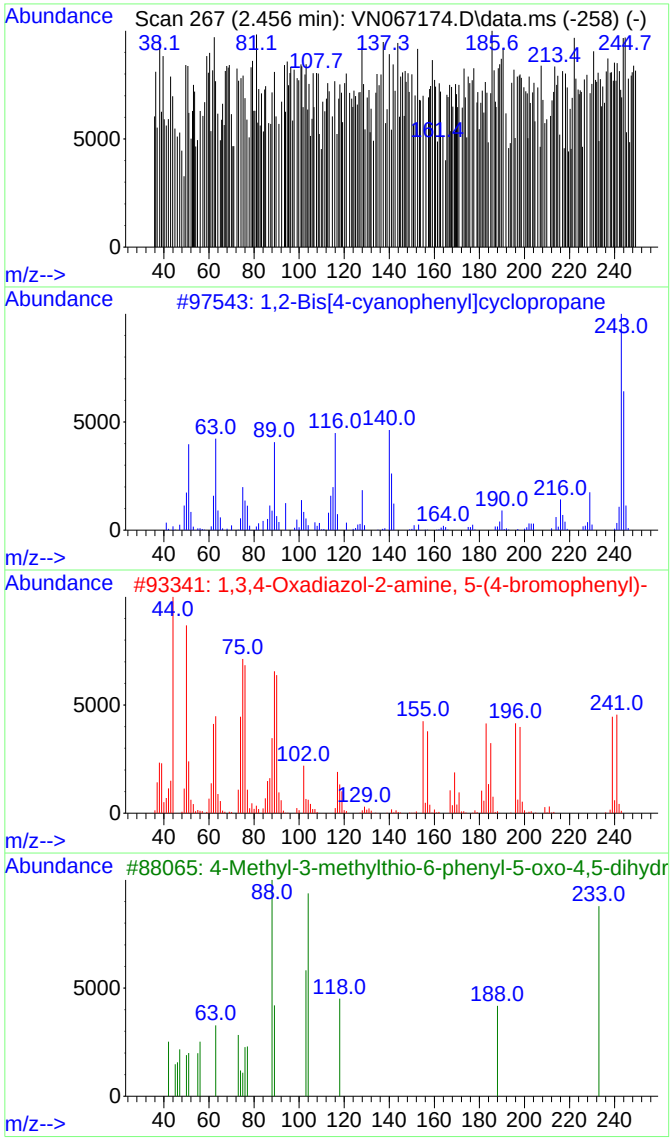
Quant Title : SW846 8260

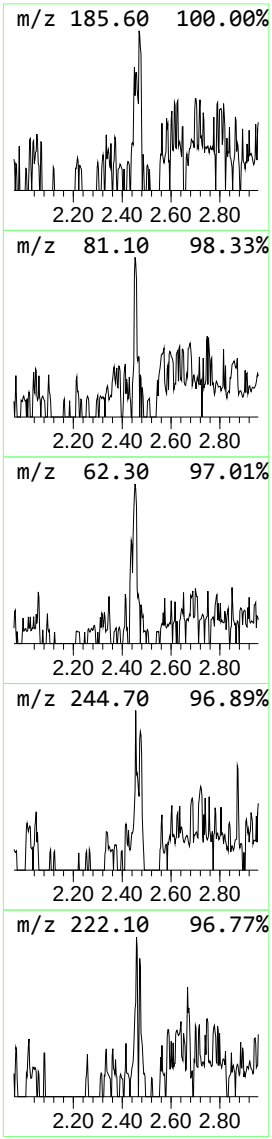
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,2-Bis[4-cyanophenyl]cyclo... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.456	21.06 ug/l	269571	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Bis[4-cyanophenyl]cyclopropane	244	C17H12N2	1000250-80-5	60
2	1,3,4-Oxadiazol-2-amine, 5-(4-br...	239	C8H6BrN3O	033621-62-4	53
3	4-Methyl-3-methylthio-6-phenyl-5...	233	C11H11N3OS	022943-30-2	53
4	2-(4-Bromophenyl)-5-methyl-[1,3,...	238	C9H7BrN2O	041421-03-8	47
5	6-Methoxy-1-methyl-8-nitro-1,2-d...	220	C11H12N2O3	059353-32-1	46





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

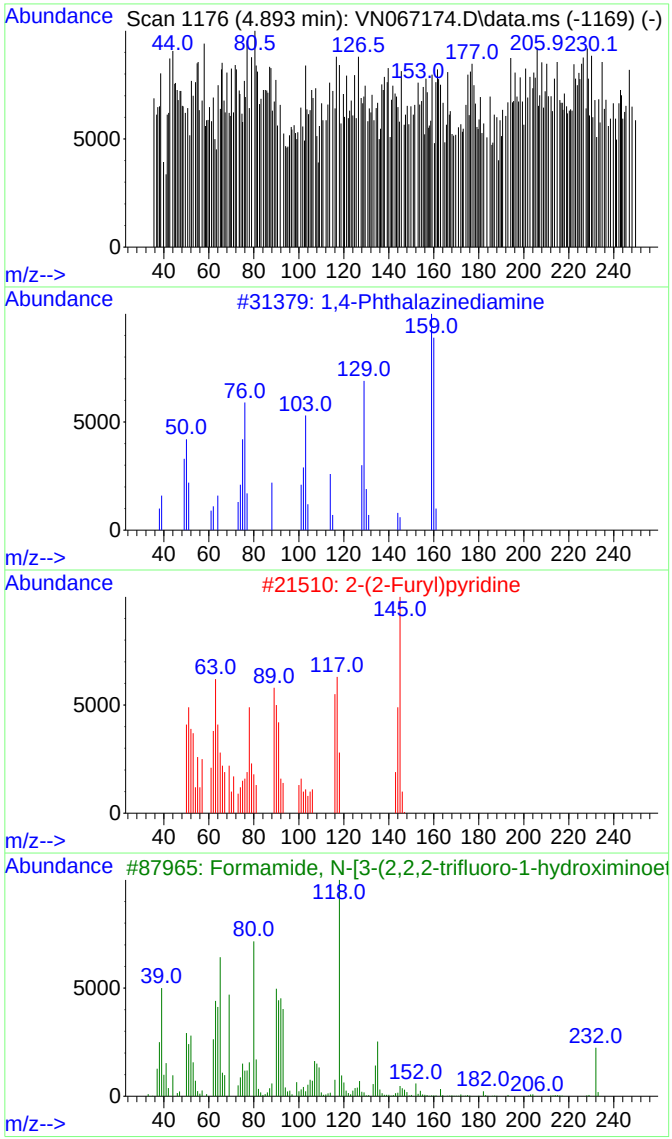
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

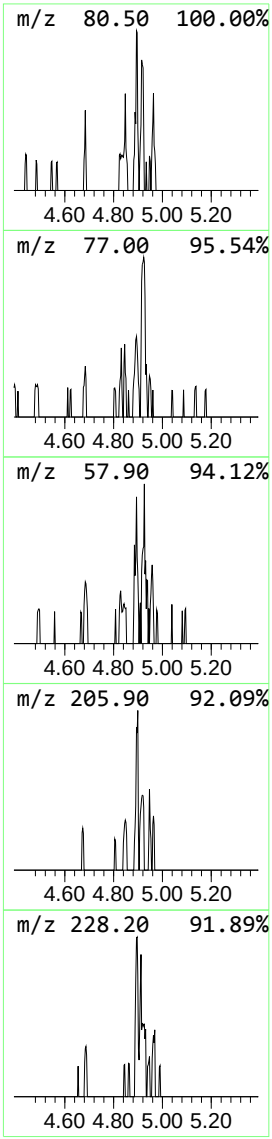
****

Peak Number 2 1,4-Phthalazinediamine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	6.91 ug/l	88508	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Phthalazinediamine	160	C8H8N4	017987-70-1	91
2	2-(2-Furyl)pyridine	145	C9H7NO	055484-03-2	90
3	Formamide, N-[3-(2,2,2-trifluoro...	232	C9H7F3N2O2	079684-38-1	68
4	4-Amino-5,7-dinitrobenzofurazan	225	C6H3N5O5	021123-74-0	62
5	Benzenamine, 4-(2-methoxyphenoxy)-	215	C13H13NO2	1000362-56-7	62





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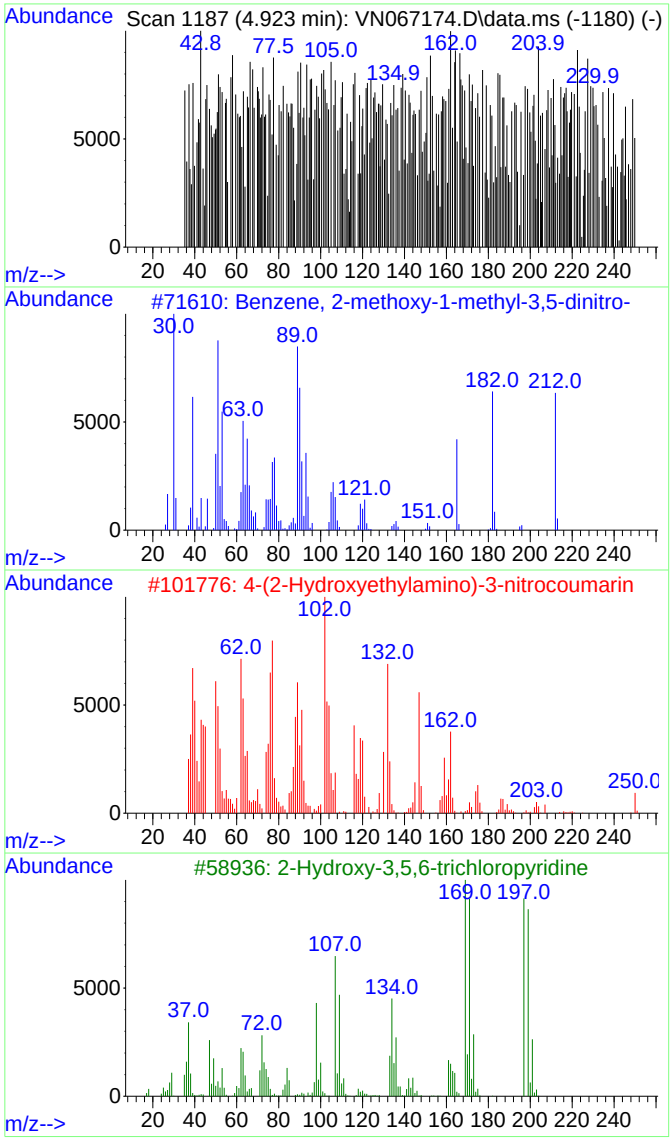
Quant Title : SW846 8260

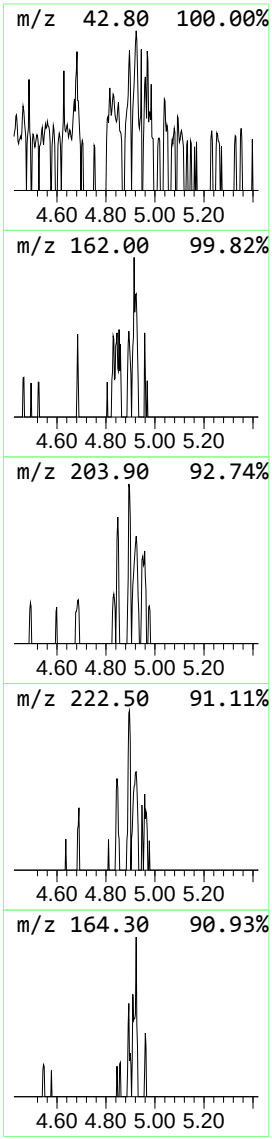
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 2-methoxy-1-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.923	10.61 ug/l	135817	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-methoxy-1-methyl-3,5-...	212	C8H8N2O5	029027-13-2	64
2	4-(2-Hydroxyethylamino)-3-nitroc...	250	C11H10N2O5	088353-20-2	56
3	2-Hydroxy-3,5,6-trichloropyridine	197	C5H2Cl3NO	006515-38-4	56
4	1,3-Benzodioxole-5-carboxaldehyd...	210	C10H10O5	1000362-70-0	55
5	2-Phenyl-3-(4-fluorophenyl)-oxirane	214	C14H11FO	1000147-27-7	46





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TIC Library : C:\DATABASE\NIST11.L
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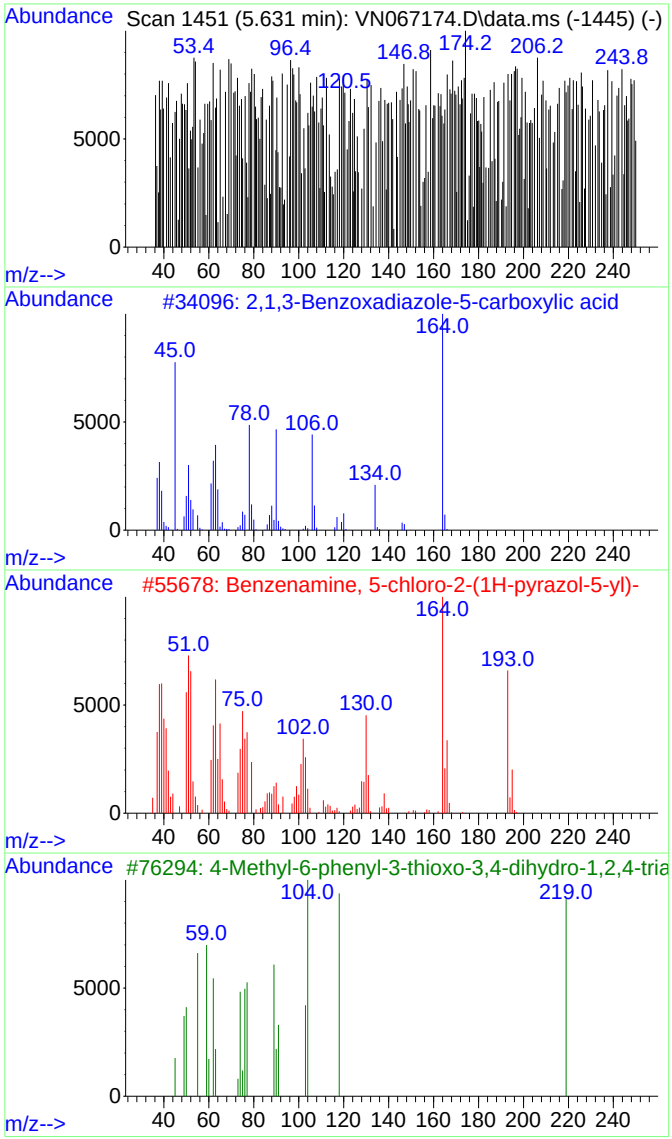
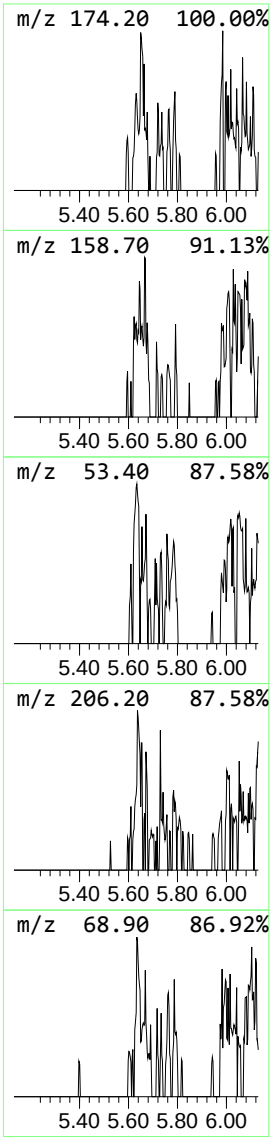
****
Peak Number 4 2,1,3-Benzoxadiazole-5-carb... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.631	7.11 ug/l	91047	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,1,3-Benzoxadiazole-5-carboxyli...	164	C7H4N2O3	1000351-32-1	55
2	Benzenamine, 5-chloro-2-(1H-pyra...	193	C9H8ClN3	1000362-66-8	53
3	4-Methyl-6-phenyl-3-thioxo-3,4-d...	219	C10H9N3OS	022936-87-4	47
4	Norcaranoic acid, methyl ester, ...	154	C9H14O2	1000149-95-2	45
5	Phenol, 2,3,6-trichloro-	196	C6H3Cl3O	000933-75-5	45





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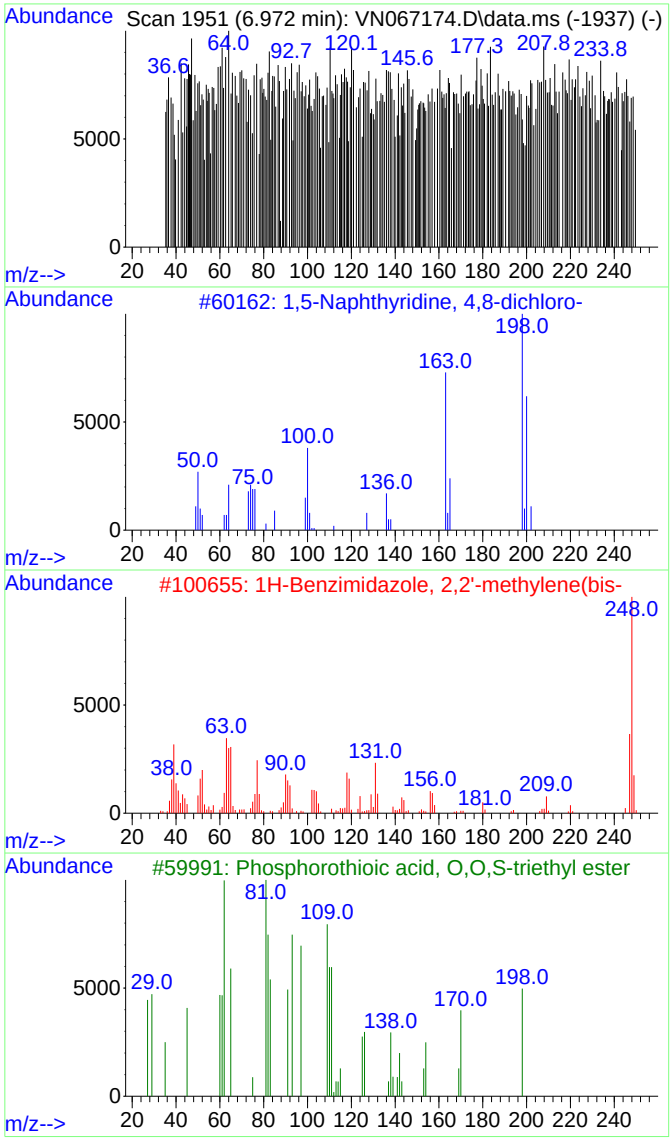
Quant Title : SW846 8260

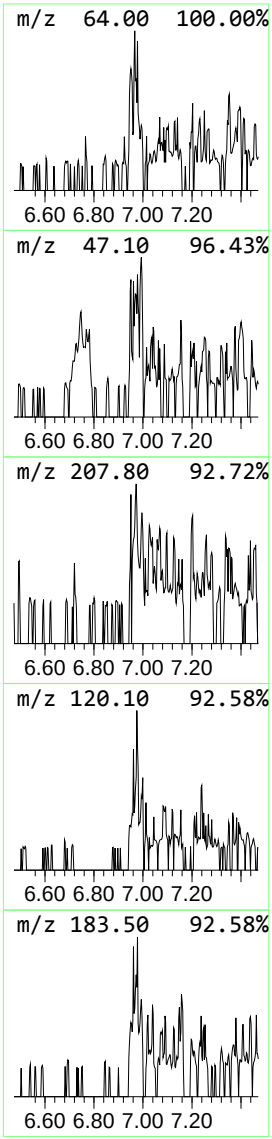
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,5-Naphthyridine, 4,8-dich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.972	19.87 ug/l	254332	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Naphthyridine, 4,8-dichloro-	198	C8H4Cl2N2	028252-80-4	55
2	1H-Benzimidazole, 2,2'-methylene...	248	C15H12N4	005999-14-4	55
3	Phosphorothioic acid, O,O,S-trie...	198	C6H15O3PS	001186-09-0	55
4	1,5-Naphthyridine, 3,8-dichloro-	198	C8H4Cl2N2	028252-81-5	53
5	Furazan-3-carbohydrazide, 4-amin...	232	C9H8N6O2	1000264-22-7	51





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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41791

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

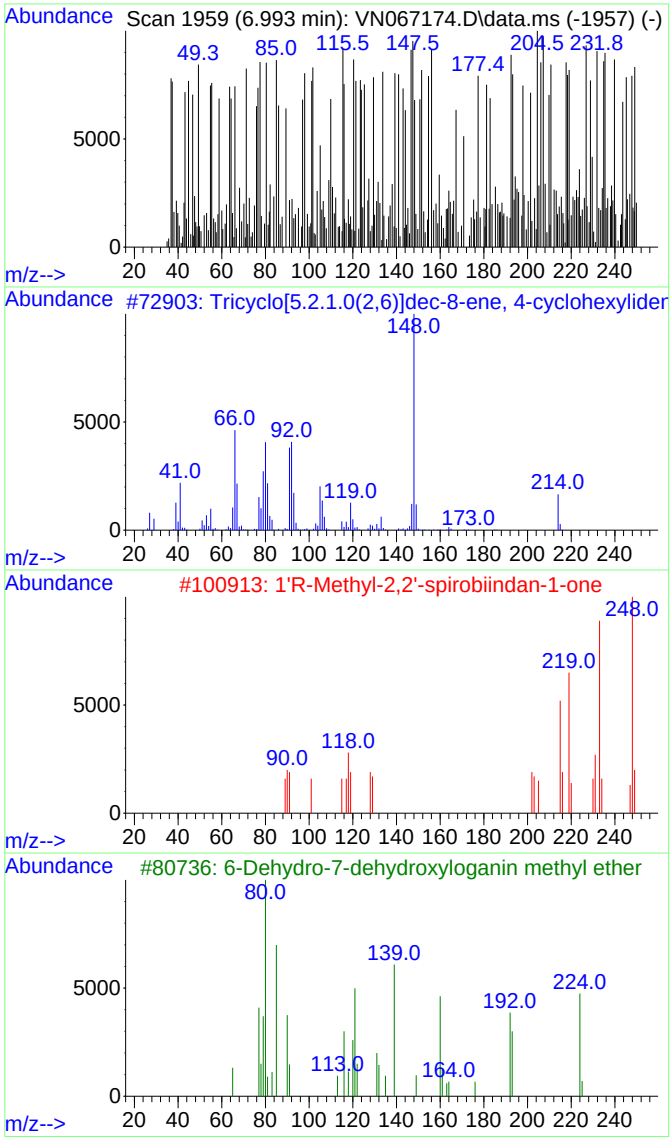
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

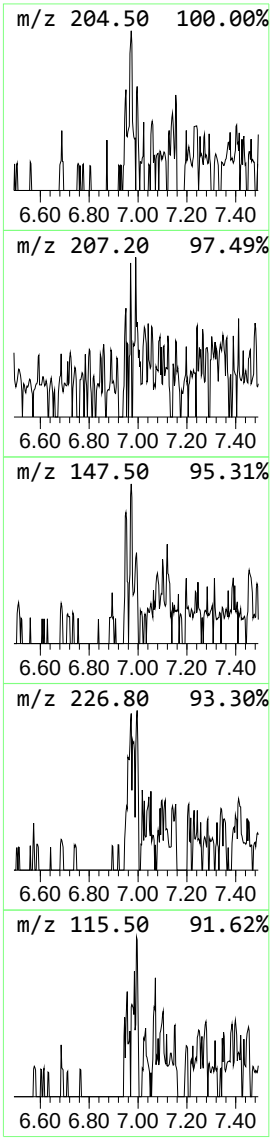
****

Peak Number 6 unknown6.993 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.993	5.66 ug/l	72516	Pentafluorobenzene	7.597

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.1.0(2,6)]dec-8-ene,...	214	C16H22	1000154-22-4	18
2	1'R-Methyl-2,2'-spirobiindan-1-one	248	C18H16O	082309-97-5	15
3	6-Dehydro-7-dehydroxyloganin met...	224	C12H16O4	023661-16-7	15
4	Morpholine, 4-(1,3-butadienyl)-	139	C8H13NO	019352-93-3	14
5	1H-Cyclopenta[b]quinoxalin-1-one...	214	C11H6N2O3	023774-23-4	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067174.D
Acq On : 26 May 2021 18:05
Operator : JC/MD
Sample : M2529-02 50X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41791

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
1,2-Bis[4-cyano...	2.456	21.1	ug/l	269571	1	7.597	640077	50.0
1,4-Phthalazine...	4.893	6.9	ug/l	88508	1	7.597	640077	50.0
Benzene, 2-meth...	4.923	10.6	ug/l	135817	1	7.597	640077	50.0
2,1,3-Benzoxadi...	5.631	7.1	ug/l	91047	1	7.597	640077	50.0
1,5-Naphthyridi...	6.972	19.9	ug/l	254332	1	7.597	640077	50.0
unknown6.993	6.993	5.7	ug/l	72516	1	7.597	640077	50.0