

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
 Data File : VN067175.D
 Acq On : 26 May 2021 18:28
 Operator : JC/MD
 Sample : M2529-03 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41822

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: VN067175.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.415	243	252	260	rBV	61616	103067	7.88%	1.438%
2	2.474	270	274	278	rVB6	29187	20334	1.55%	0.284%
3	2.512	282	288	293	rBV9	28831	20606	1.57%	0.287%
4	2.579	308	313	317	rBV7	31541	25506	1.95%	0.356%
5	2.649	337	339	346	rVB7	51169	41390	3.16%	0.577%
6	2.676	346	349	353	rBV5	31437	20805	1.59%	0.290%
7	2.761	374	381	385	rBV6	50555	37094	2.84%	0.517%
8	2.810	391	399	403	rBV8	50550	73862	5.65%	1.030%
9	2.836	403	409	419	rVV8	35137	73850	5.64%	1.030%
10	3.013	470	475	478	rBV5	30090	16060	1.23%	0.224%
11	3.038	478	484	489	rVB7	40683	33864	2.59%	0.472%
12	3.641	705	709	715	rBV8	28330	36173	2.76%	0.505%
13	7.516	2129	2154	2168	rBV2	158021	406350	31.06%	5.668%
14	7.597	2169	2184	2199	rVV2	268869	632744	48.36%	8.825%
15	7.645	2199	2202	2206	rVB5	25075	13543	1.04%	0.189%
16	7.712	2223	2227	2234	rVB6	51108	46399	3.55%	0.647%
17	7.959	2296	2319	2346	rBV	187238	460926	35.23%	6.429%
18	8.522	2510	2529	2558	rBV	454530	996695	76.18%	13.901%
19	10.035	3075	3093	3114	rBV	669020	1308388	100.00%	18.249%
20	11.360	3570	3587	3633	rBV	566995	1120623	85.65%	15.630%
21	12.360	3942	3960	4020	rBV	272480	728744	55.70%	10.164%
22	13.301	4296	4311	4351	rBV	327110	860549	65.77%	12.002%
23	15.224	5020	5028	5031	rBV9	15030	15299	1.17%	0.213%
24	15.329	5059	5067	5072	rVB9	17978	21541	1.65%	0.300%
25	15.383	5080	5087	5089	rBV6	39884	34010	2.60%	0.474%
26	15.525	5136	5140	5146	rVV7	27981	21330	1.63%	0.297%

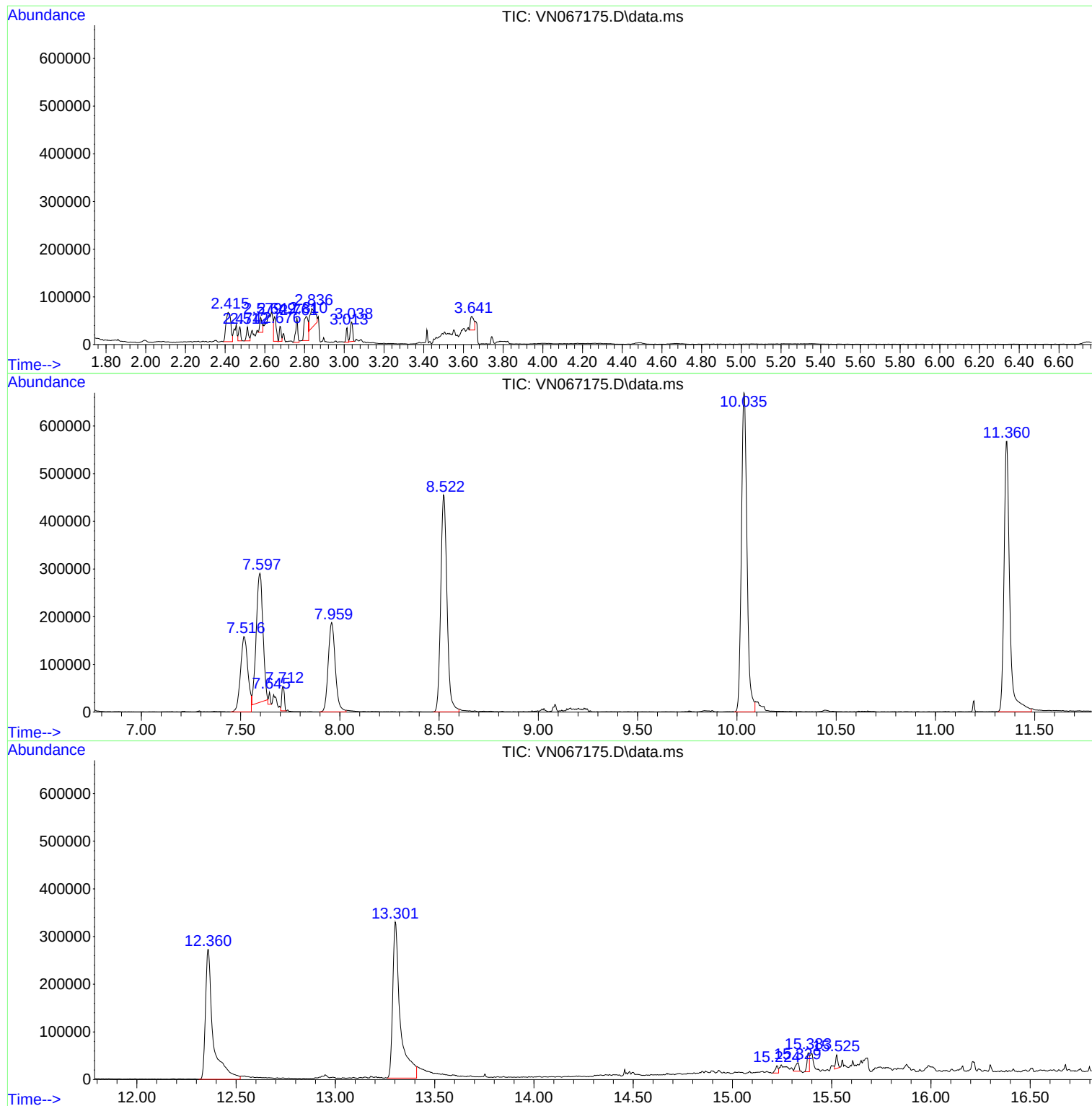
Sum of corrected areas: 7169752

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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



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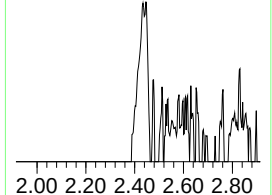
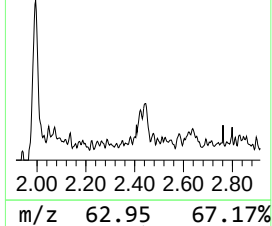
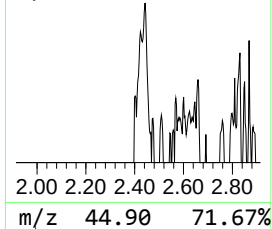
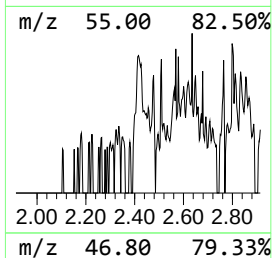
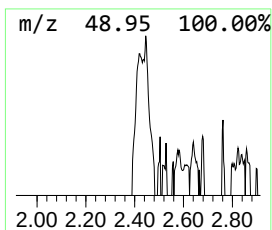
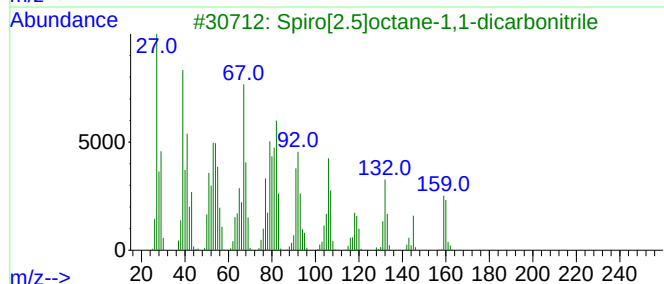
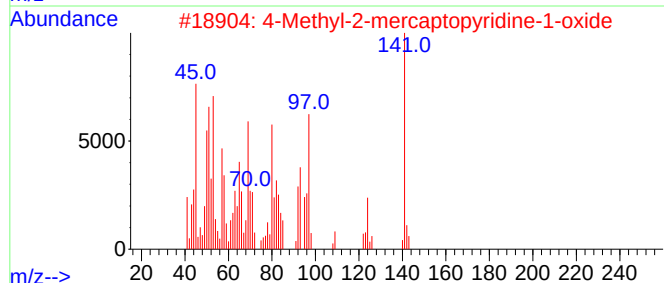
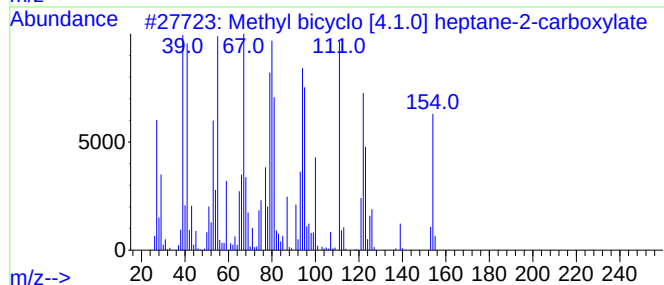
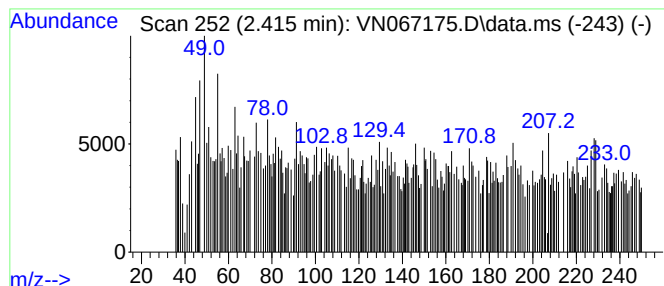
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.415 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.415	8.14 ug/l	103067	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl bicyclo [4.1.0] heptane-2...	154	C9H14O2	1000222-05-0	44
2			4-Methyl-2-mercaptopyridine-1-oxide	141	C6H7NOS	034341-26-9	38
3			Spiro[2.5]octane-1,1-dicarbonitrile	160	C10H12N2	068352-24-9	38
4			4-Nitro-2-picoline N-oxide	154	C6H6N2O3	005470-66-6	35
5			1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	000694-31-5	25



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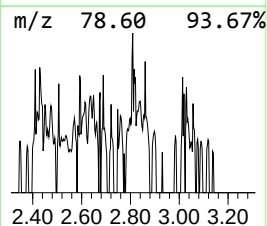
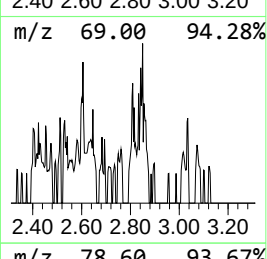
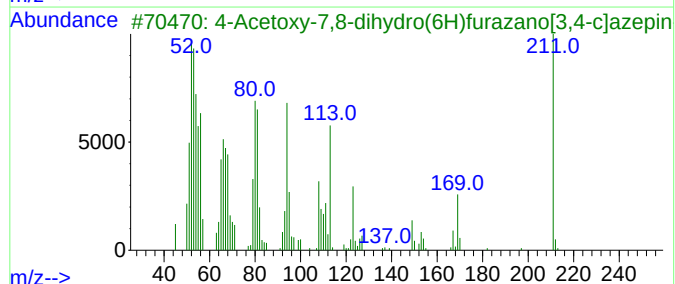
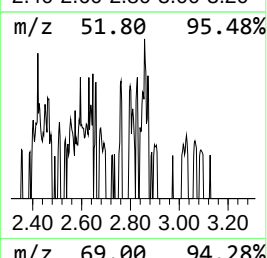
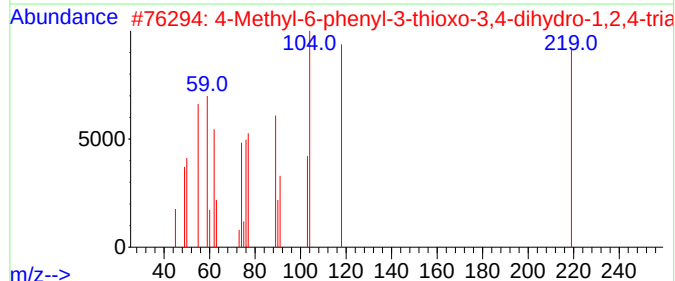
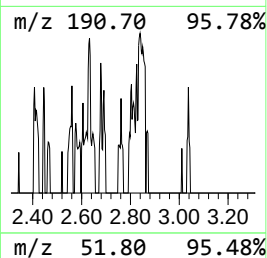
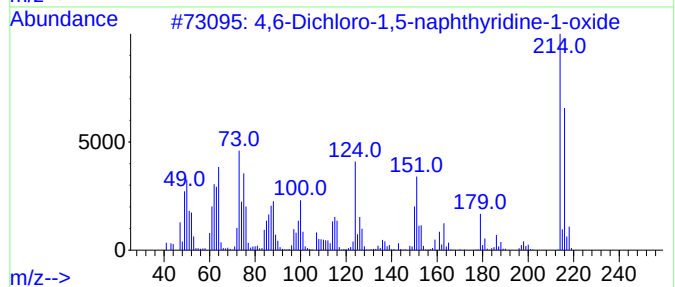
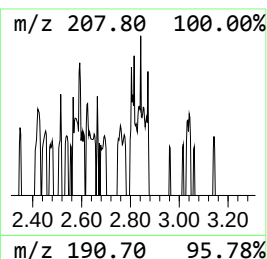
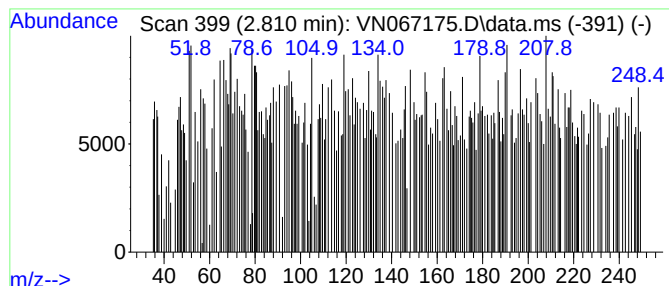
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Peak Number 2 4,6-Dichloro-1,5-naphthyrid... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.810	5.84 ug/l	73862	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,6-Dichloro-1,5-naphthyridine-1...	214	C8H4Cl2N2O	1000213-90-4	89
2			4-Methyl-6-phenyl-3-thioxo-3,4-d...	219	C10H9N3OS	022936-87-4	53
3			4-Acetoxy-7,8-dihydro(6H)furazan...	211	C8H9N3O4	1000110-73-8	47
4			Pyridazine, 3,6-dichloro-4-methyl-	162	C5H4Cl2N2	019064-64-3	41
5			Benzenethiol, 2,4-dichloro-	178	C6H4Cl2S	001122-41-4	38



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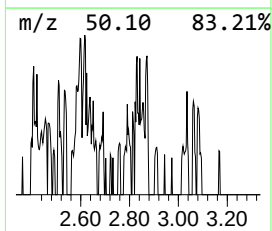
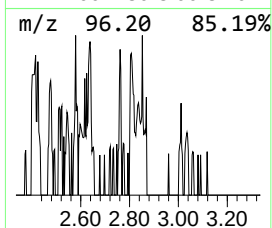
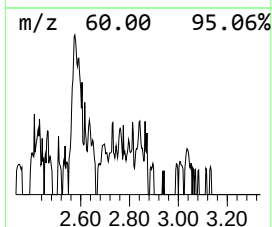
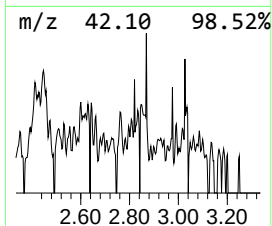
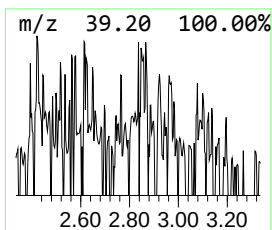
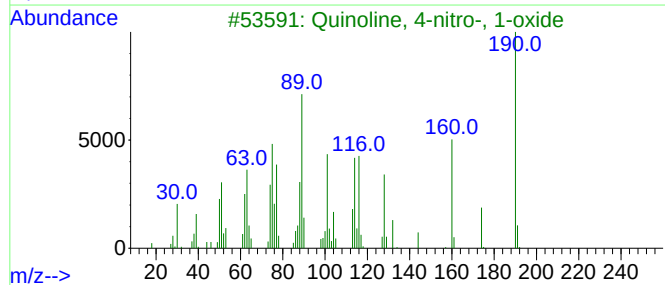
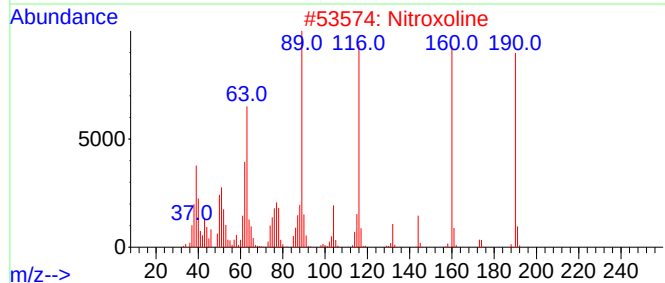
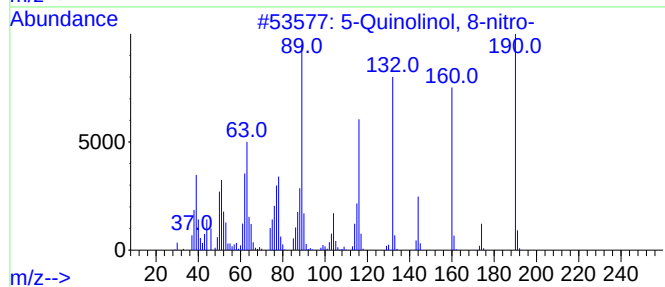
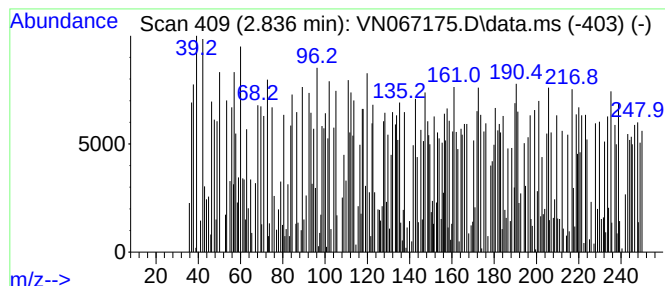
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Quant Title : SW846 8260

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

Peak Number 3 unknown2.836 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.836	5.84 ug/l	73850	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Quinolinol, 8-nitro-			190	C9H6N2O3	1000319-80-0	40
2	Nitroxoline			190	C9H6N2O3	004008-48-4	25
3	Quinoline, 4-nitro-, 1-oxide			190	C9H6N2O3	000056-57-5	25
4	Sulphamide, N-(4-nitrophenyl)-			217	C6H7N3O4S	070466-80-7	25
5	3-Benzofurancarboxylic acid			162	C9H6O3	026537-68-8	25



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.415	2.415	8.1	ug/l	103067	1	7.597	632744	50.0
4,6-Dichloro-1,...	2.810	5.8	ug/l	73862	1	7.597	632744	50.0
unknown2.836	2.836	5.8	ug/l	73850	1	7.597	632744	50.0