

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
 Data File : VN067176.D
 Acq On : 26 May 2021 18:52
 Operator : JC/MD
 Sample : M2529-04 50X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41815

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: VN067176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.131	139	146	151	rBV8	23675	27549	1.48%	0.257%
2	2.166	151	159	164	rVV9	33601	47151	2.53%	0.440%
3	2.201	168	172	179	rBV9	28289	22249	1.19%	0.208%
4	2.300	195	209	227	rBV	109862	199266	10.68%	1.859%
5	2.912	429	437	446	rVB	48039	67842	3.64%	0.633%
6	3.306	572	584	587	rBV	87430	172246	9.23%	1.607%
7	3.325	587	591	598	rVB10	68001	75736	4.06%	0.707%
8	3.577	682	685	692	rBV8	25963	21964	1.18%	0.205%
9	3.612	693	698	705	rVB8	22599	28323	1.52%	0.264%
10	4.593	1059	1064	1065	rBV4	38046	21523	1.15%	0.201%
11	5.398	1353	1364	1365	rBV10	106063	151218	8.10%	1.411%
12	5.814	1515	1519	1523	rBV4	46982	31302	1.68%	0.292%
13	5.851	1524	1533	1536	rBV8	57475	78932	4.23%	0.736%
14	5.913	1553	1556	1559	rBV4	27723	19528	1.05%	0.182%
15	5.964	1569	1575	1587	rVB4	29608	40638	2.18%	0.379%
16	6.033	1597	1601	1607	rVB7	69169	44274	2.37%	0.413%
17	6.243	1673	1679	1687	rVB9	138783	172317	9.23%	1.608%
18	6.406	1732	1740	1744	rBV10	18957	25561	1.37%	0.238%
19	6.591	1803	1809	1815	rBV10	37775	35834	1.92%	0.334%
20	6.715	1845	1855	1856	rBV9	21788	26950	1.44%	0.251%
21	6.948	1936	1942	1955	rVB9	24240	38160	2.04%	0.356%
22	7.173	2020	2026	2037	rBV9	25044	39089	2.09%	0.365%
23	7.514	2139	2153	2169	rBV2	215422	536012	28.72%	5.001%
24	7.594	2170	2183	2206	rVV	381125	904916	48.49%	8.442%
25	7.669	2206	2211	2217	rVB9	20595	22853	1.22%	0.213%
26	7.959	2299	2319	2335	rBV	279787	732886	39.27%	6.837%
27	8.522	2512	2529	2555	rVV	600316	1322201	70.85%	12.335%
28	9.067	2726	2732	2742	rBV	23237	31719	1.70%	0.296%
29	10.035	3074	3093	3110	rBV	981864	1866131	100.00%	17.410%
30	11.357	3572	3586	3608	rBV	760759	1411700	75.65%	13.170%
31	12.202	3890	3901	3903	rBV	16523	19630	1.05%	0.183%
32	12.358	3945	3959	3979	rBV	466331	990951	53.10%	9.245%
33	12.926	4166	4171	4176	rVB8	28171	26204	1.40%	0.244%
34	12.977	4185	4190	4191	rBV5	34335	21773	1.17%	0.203%
35	13.213	4273	4278	4281	rBV6	34232	31123	1.67%	0.290%
36	13.299	4294	4310	4335	rBV	580346	1342127	71.92%	12.521%

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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

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Title : SW846 8260

37	14.519	4760	4765	4767	rBV6	32466	25040	1.34%	0.234%
38	14.857	4884	4891	4894	rBV8	19235	22842	1.22%	0.213%
39	15.898	5276	5279	5285	rVB7	33336	23196	1.24%	0.216%

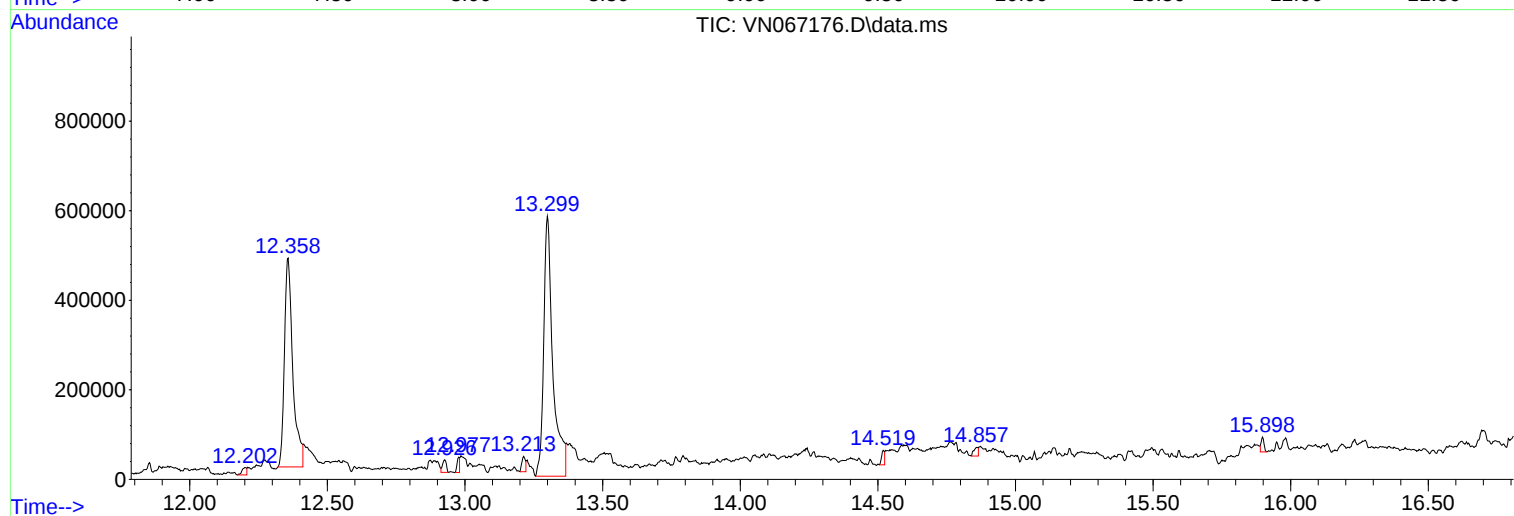
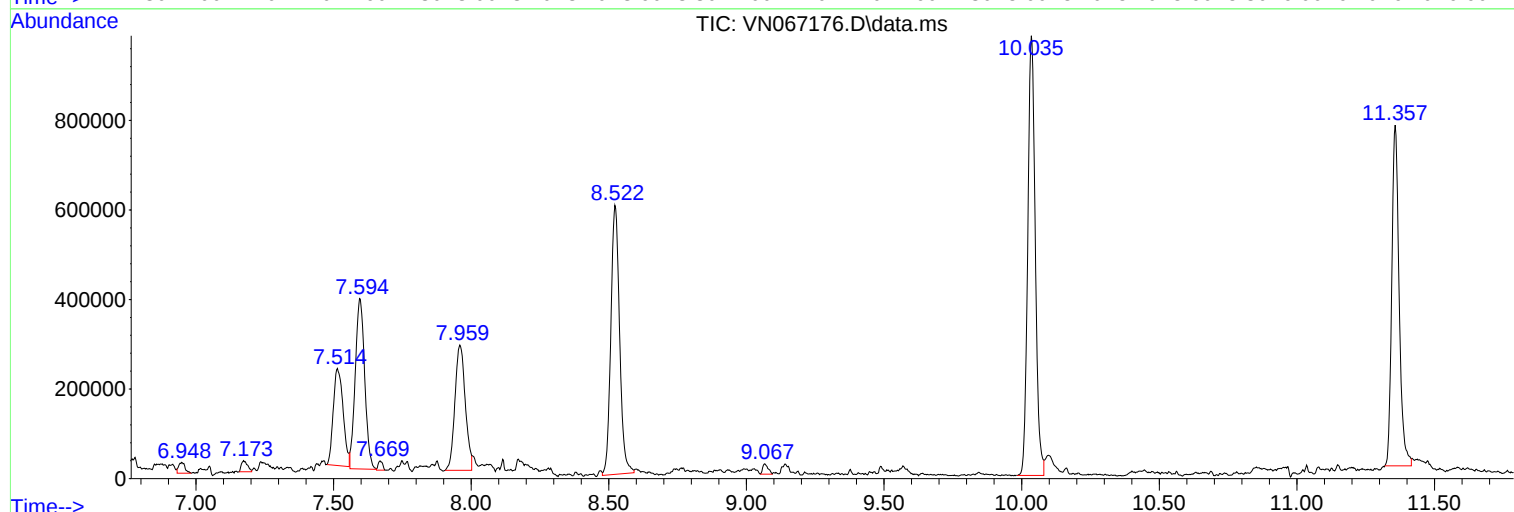
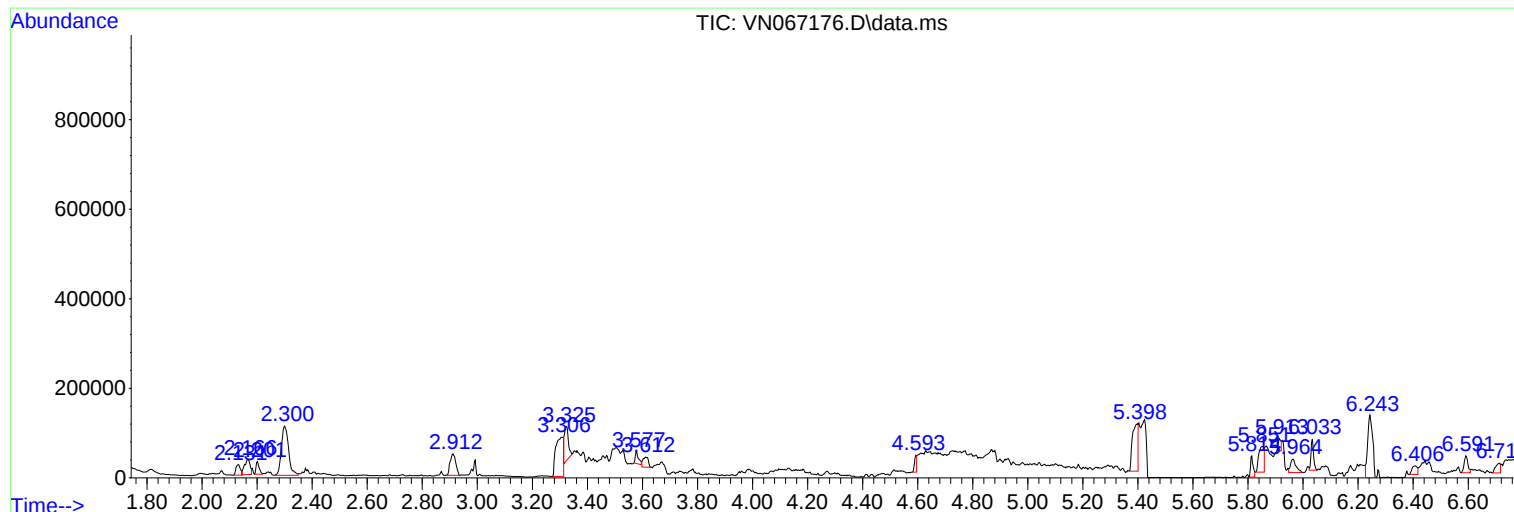
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

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



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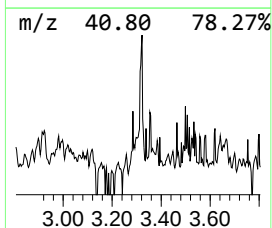
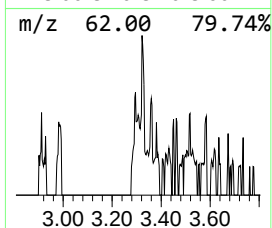
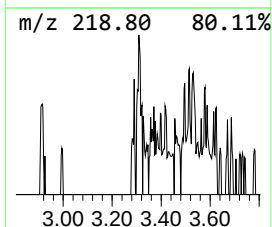
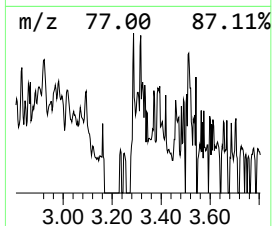
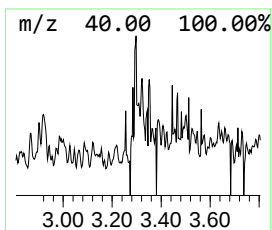
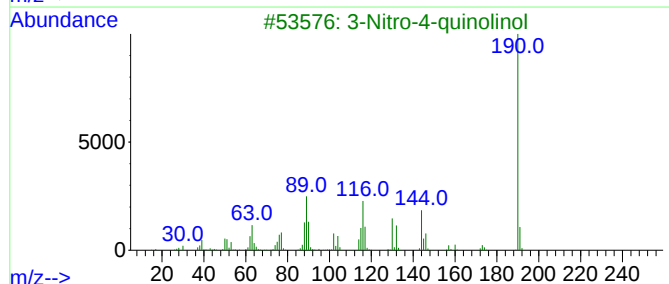
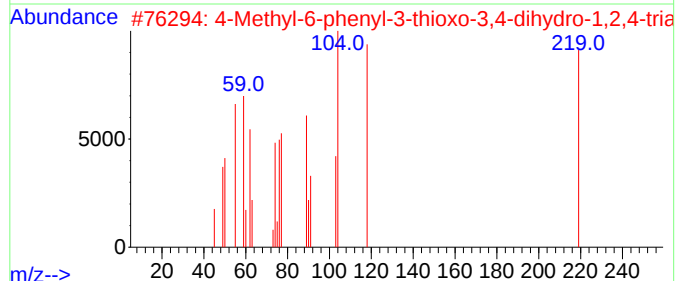
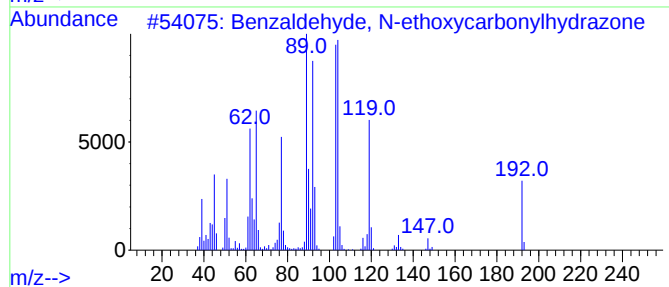
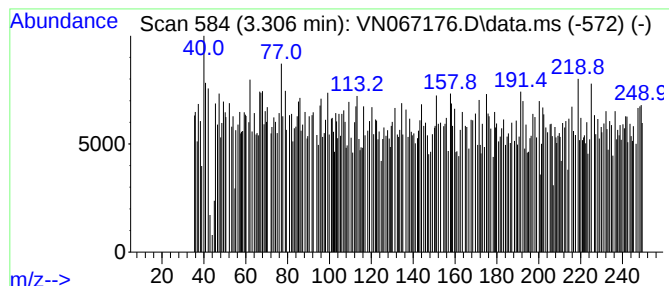
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzaldehyde, N-ethoxycarbo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.306	9.52 ug/l	172246	Pentafluorobenzene	7.594

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, N-ethoxycarbonylhy...	192	C10H12N2O2	016208-36-9	83
2			4-Methyl-6-phenyl-3-thioxo-3,4-d...	219	C10H9N3OS	022936-87-4	64
3			3-Nitro-4-quinolinol	190	C9H6N2O3	050332-66-6	59
4			2-Imino-6-nitro-2H-1-benzopyran-...	249	C10H7N3O3S	1000223-66-6	47
5			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	45



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Instrument :
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ClientSampleId :
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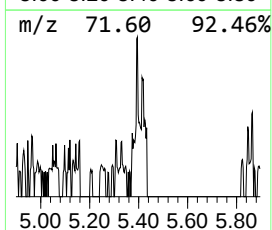
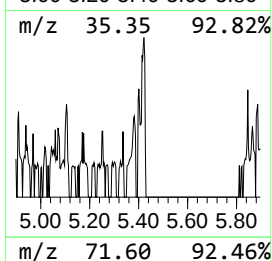
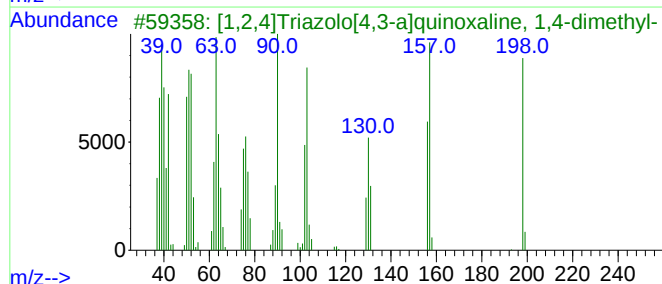
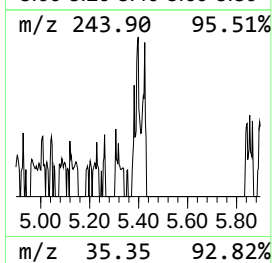
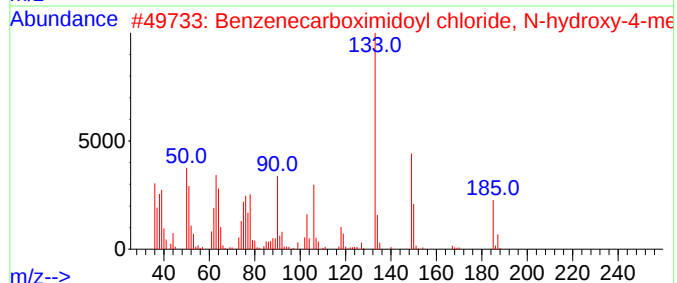
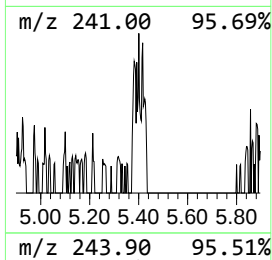
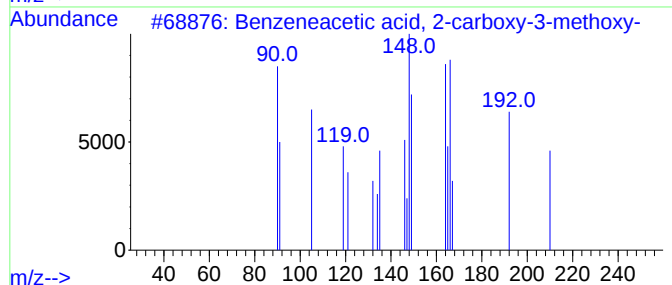
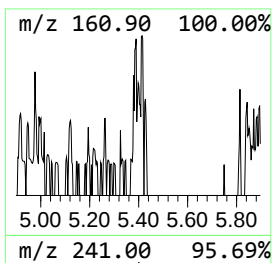
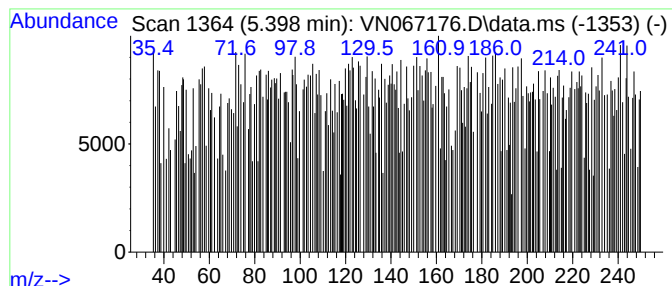
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Quant Title : SW846 8260

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

Peak Number 3 Benzeneacetic acid, 2-carbo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.398	8.36 ug/l	151218	Pentafluorobenzene	7.594

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid, 2-carboxy-3-...	210	C10H10O5	001137-31-1	83
2			Benzenecarboximidoyl chloride, N...	185	C8H8ClNO2	1000362-64-9	78
3			[1,2,4]Triazolo[4,3-a]quinoxalin...	198	C11H10N4	1000362-67-9	59
4			4-Quinolinesulfonamide 1-oxide	224	C9H8N2O3S	1000241-86-5	58
5			4-(2-Hydroxyethylamino)-3-nitroc...	250	C11H10N2O5	088353-20-2	58



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ClientSampled :
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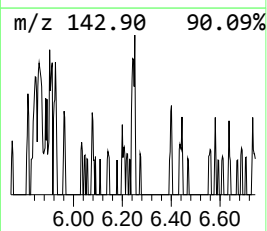
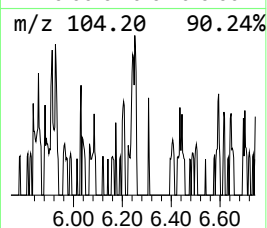
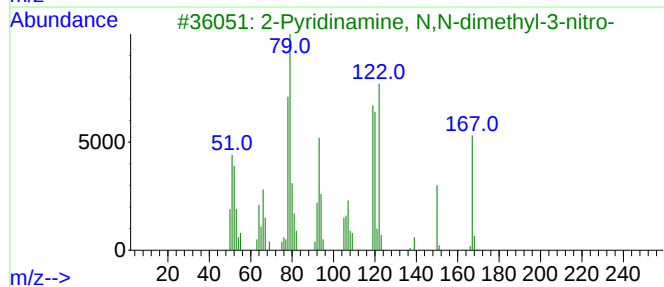
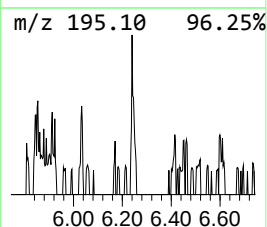
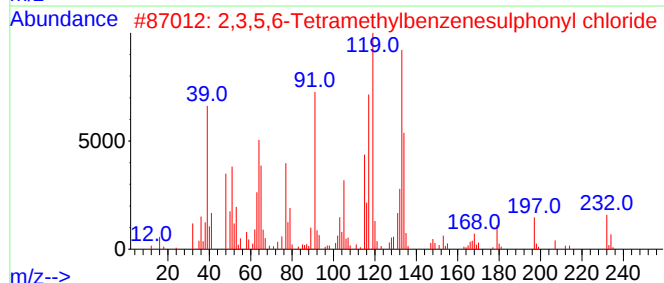
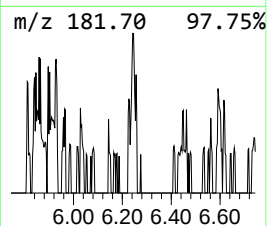
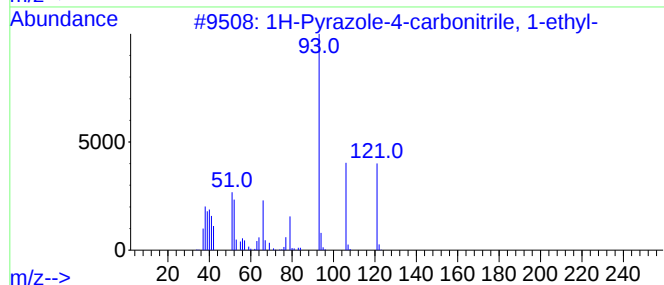
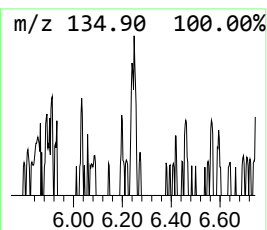
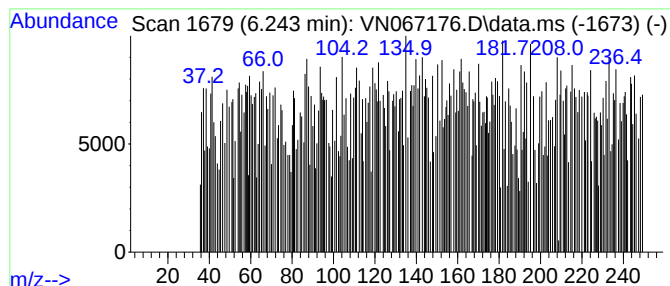
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Quant Title : SW846 8260

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

Peak Number 4 1H-Pyrazole-4-carbonitrile,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.243	9.52 ug/l	172317	Pentafluorobenzene	7.594

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole-4-carbonitrile, 1-et...	121	C6H7N3	1000351-26-5	72
2			2,3,5,6-Tetramethylbenzenesulpho...	232	C10H13ClO2S	1000342-51-8	55
3			2-Pyridinamine, N,N-dimethyl-3-n...	167	C7H9N3O2	005028-23-9	52
4			Acetyl chloride, (2,4-dichloroph...	238	C8H5Cl3O2	000774-74-3	48
5			Benzoic acid, 4-(2-hydroxyimino...	236	C11H12N2O4	017122-79-1	45



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzaldehyde, N...	3.306	9.5	ug/l	172246	1	7.594	904916	50.0
Benzeneacetic a...	5.398	8.4	ug/l	151218	1	7.594	904916	50.0
1H-Pyrazole-4-c...	6.243	9.5	ug/l	172317	1	7.594	904916	50.0