LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN052621\
Data File : VN067172.D
Acq On : 26 May 2021 17:18
Operator : JC/MD
Sample : M2518-05 200X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 118-119

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: VN067172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.421	246	254	255	rBV5	89576	88079	4.80%	0.573%
2	2.466	265	271	275	rBV7	68256	77083	4.20%	0.501%
3	2.482	275	277	282	rVV6	65209	52563	2.87%	0.342%
4	2.504	282	285	289	rVV6	59595	40012	2.18%	0.260%
5	2.598	313	320	324	rVB8	23815	19021	1.04%	0.124%
6	2.651	330	340	344	rBV8	79416	95469	5.21%	0.621%
7	2.686	349	353	364	rVB8	55449	60900	3.32%	0.396%
8	2.748	372	376	383	rBV8	22625	25134	1.37%	0.163%
9	2.796	390	394	396	rBV4	24427	18974	1.03%	0.123%
10	2.973	447	460	464	rBV4	66493	97735	5.33%	0.635%
11	2.995	464	468	476	rVV10	38183	51568	2.81%	0.335%
12	3.067	492	495	498	rBV5	44934	28477	1.55%	0.185%
13	3.126	515	517	521	rVB4	43863	19422	1.06%	0.126%
14	3.279	570	574	578	rBV5	60280	64815	3.53%	0.421%
15	3.357	598	603	607	rBV5	32522	19396	1.06%	0.126%
16	3.531	664	668	670	rBV2	46271	28303	1.54%	0.184%
17	3.762	741	754	768	rBV	214096	475729	25.94%	3.092%
18	3.858	784	790	791	rBV5	33620	25306	1.38%	0.164%
19	4.116	882	886	889	rBV5	32289	18872	1.03%	0.123%
20	4.228	924	928	933	rVB5	23205	20221	1.10%	0.131%
21	4.480	999	1022	1063	rVB2	299622	1001841	54.64%	6.512%
22	5.459	1383	1387	1389	rVV3	45858	24457	1.33%	0.159%
23	5.679	1461	1469	1474	rVB9	46358	50731	2.77%	0.330%
24	5.754	1489	1497	1505	rVB9	67097	87296	4.76%	0.567%
25	5.813	1514	1519	1521	rBV5	60026	48629	2.65%	0.316%
26	6.025	1592	1598	1608	rVB5	50630	70704	3.86%	0.460%
27	6.065	1608	1613	1616	rBV5	53814	59428	3.24%	0.386%
28	6.181	1653	1656	1658	rBV4	34501	19540	1.07%	0.127%
29	6.205	1662	1665	1668	rVB4	42562	24818	1.35%	0.161%
30	6.229	1668	1674	1676	rBV5	37239	39112	2.13%	0.254%
31	6.250	1676	1682	1684	rBV7	27715	21339	1.16%	0.139%
32	6.897	1914	1923	1927	rVB6	35215	34472	1.88%	0.224%
33	7.516	2130	2154	2169	rBV2	201516	533795	29.11%	3.470%
34	7.594	2169	2183	2205	rVB	327249	809392	44.14%	5.261%
35	7.790	2251	2256	2276	rVB7	30244	33309	1.82%	0.217%
36	7.959	2295	2319	2350	rBV	240494	594798	32.44%	3.866%

LSC Area Percent Report

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Instrument : MSVOA_N
ClientSampleId : 118-119

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

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Title : SW846 8260

37	8.522	2510	2529	2549	rBV	537605	1169209	63.76%	7.600%
38	10.035	3072	3093	3114	rBV	874030	1674495	91.32%	10.885%
39	10.579	3276	3296	3324	rBV	388990	740229	40.37%	4.812%
40	11.000	3444	3453	3456	rBV10	37133	49580	2.70%	0.322%
41	11.357	3567	3586	3612	rBV	710806	1347216	73.47%	8.757%
42	11.464	3613	3626	3643	rVB	222052	397789	21.69%	2.586%
43	11.518	3643	3646	3649	rBV4	43455	21948	1.20%	0.143%
44	11.569	3649	3665	3693	rVV	902211	1833690	100.00%	11.919%
45	11.901	3773	3789	3820	rVB	424811	796571	43.44%	5.178%
46	12.170	3884	3889	3892	rBV6	30496	24016	1.31%	0.156%
47	12.226	3906	3910	3915	rVB7	32201	27329	1.49%	0.178%
48	12.301	3930	3938	3940	rBV9	17775	20745	1.13%	0.135%
49	12.357	3943	3959	3980	rVV	395708	858736	46.83%	5.582%
50	12.497	4003	4011	4015	rBV10	35841	45716	2.49%	0.297%
51	12.795	4118	4122	4129	rVV9	44056	41569	2.27%	0.270%
52	12.851	4139	4143	4149	rBV8	24283	22266	1.21%	0.145%
53	12.880	4149	4154	4166	rVB8	14738	28357	1.55%	0.184%
54	12.985	4185	4193	4195	rBV7	28574	25723	1.40%	0.167%
55	13.036	4206	4212	4216	rVB7	36479	30901	1.69%	0.201%
56	13.205	4266	4275	4277	rBV8	45523	52821	2.88%	0.343%
57	13.301	4294	4311	4326	rBV2	467626	979584	53.42%	6.368%
58	13.564	4403	4409	4415	rVB9	47893	51565	2.81%	0.335%
59	13.618	4421	4429	4442	rVB9	22441	38595	2.10%	0.251%
60	14.055	4582	4592	4597	rBV8	55599	88466	4.82%	0.575%
61	14.146	4620	4626	4627	rBV4	46451	37591	2.05%	0.244%
62	14.229	4654	4657	4661	rBV5	35725	28994	1.58%	0.188%
63	14.345	4694	4700	4701	rBV6	21787	19168	1.05%	0.125%
64	14.487	4749	4753	4765	rVB10	38206	32089	1.75%	0.209%
65	14.591	4786	4792	4797	rVB8	27623	29786	1.62%	0.194%
66	14.731	4840	4844	4847	rBV6	35792	26158	1.43%	0.170%
67	14.763	4852	4856	4860	rVB5	52127	37938	2.07%	0.247%
68	15.219	5020	5026	5029	rBV7	27348	24407	1.33%	0.159%

Sum of corrected areas: 15383987

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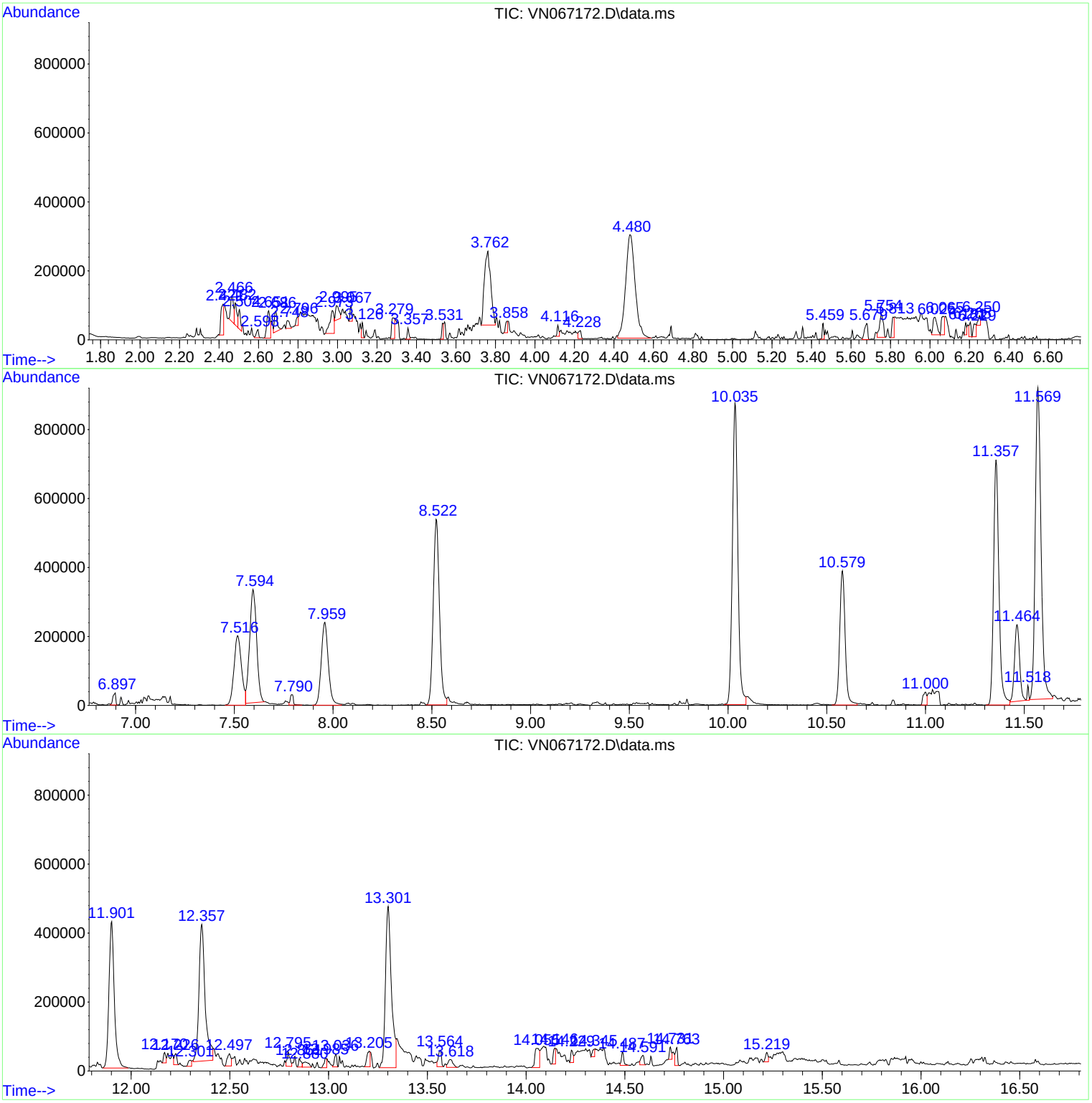
Instrument :
MSVOA_N
ClientSampleId :
118-119

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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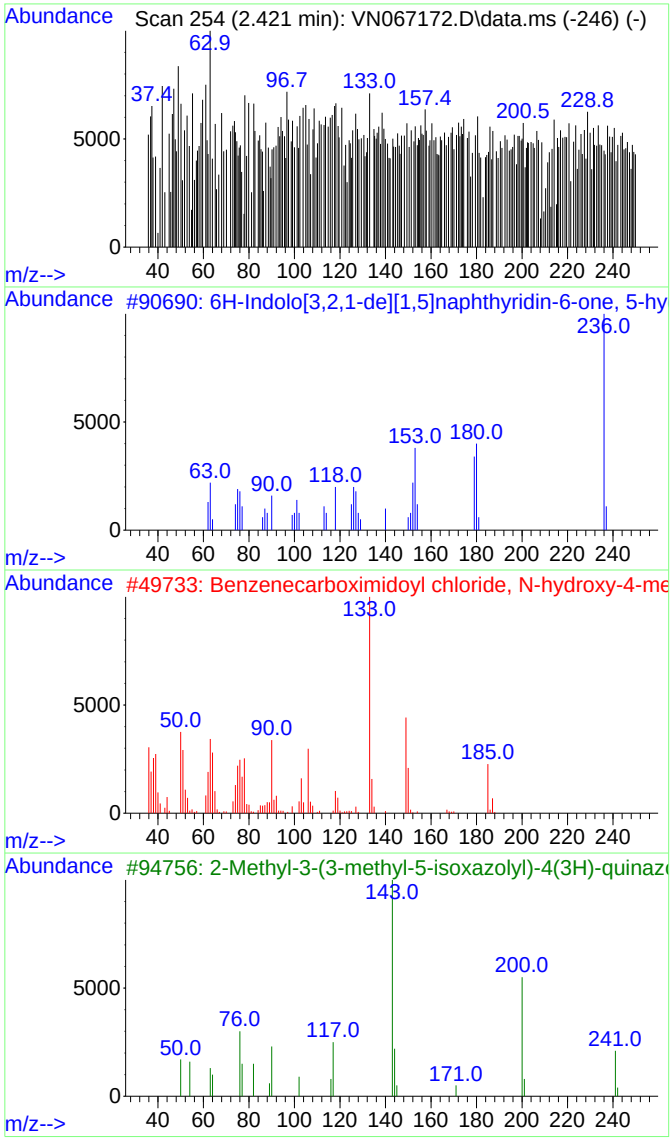
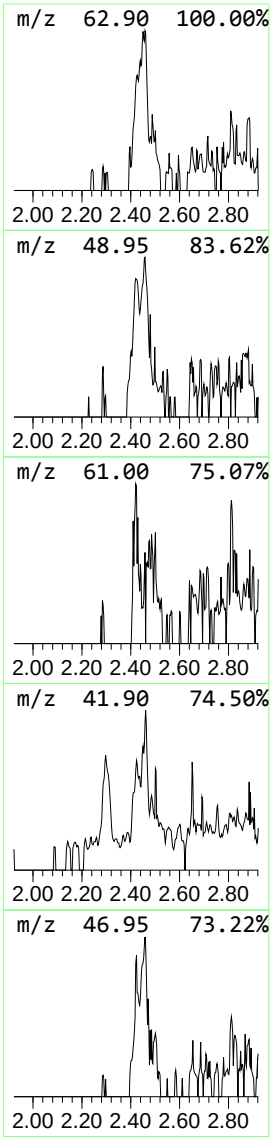
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 6H-Indolo[3,2,1-de][1,5]nap... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.421	5.44 ug/l	88079	Pentafluorobenzene	7.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Indolo[3,2,1-de][1,5]naphthyr...	236	C14H8N2O2	064118-73-6	64
2	Benzenecarboximidoyl chloride, N...	185	C8H8ClNO2	1000362-64-9	49
3	2-Methyl-3-(3-methyl-5-isoxazoly...	241	C13H11N3O2	086134-19-2	49
4	2,4,6-Trioxabicyclo[3.3.0]octane...	248	C10H16O7	076110-72-0	47
5	Quinoxaline, 2-ethyl-, 4-oxide	174	C10H10N2O	016154-83-9	46





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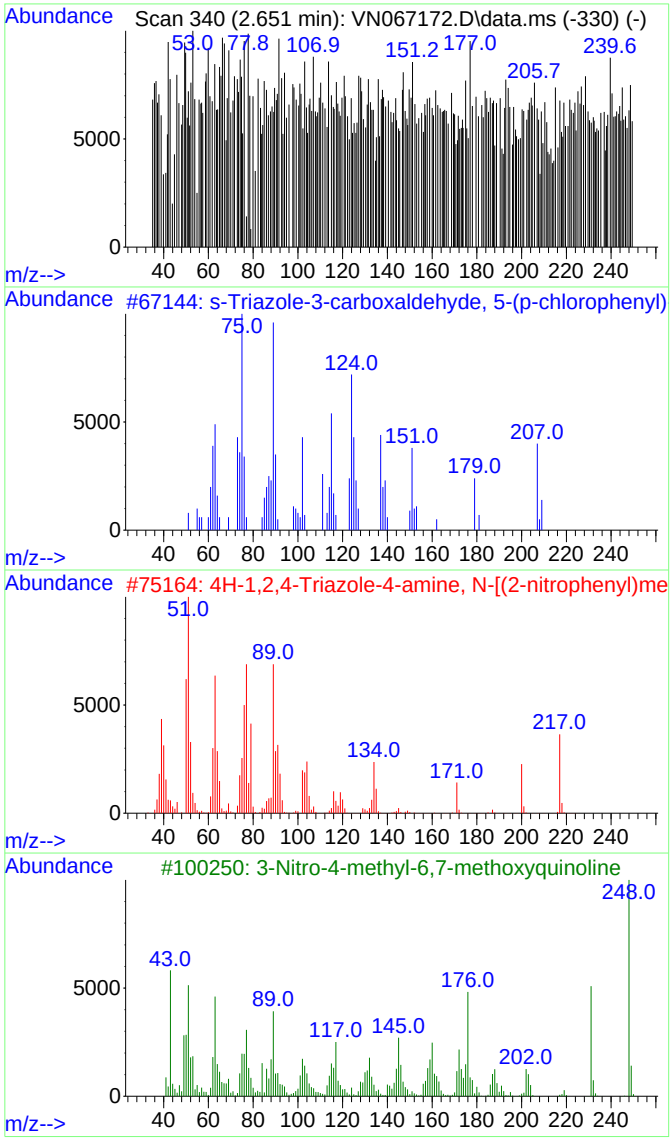
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N052121W.M
Quant Title : SW846 8260

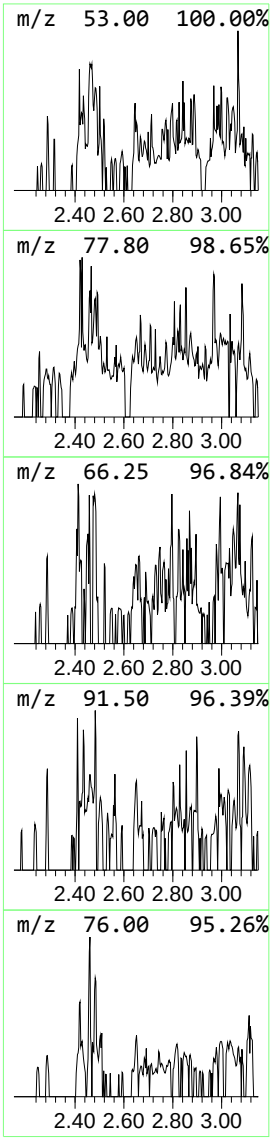
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 s-Triazole-3-carboxaldehyde... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.651	5.90 ug/l	95469	Pentafluorobenzene	7.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	s-Triazole-3-carboxaldehyde, 5-(...	207	C9H6ClN3O	026899-27-4	90
2	4H-1,2,4-Triazole-4-amine, N-[(2...	217	C9H7N5O2	035548-91-5	72
3	3-Nitro-4-methyl-6,7-methoxyquin...	248	C12H12N2O4	070945-27-6	66
4	4,5,6-Trichloro-2-benzoxazolinone	237	C7H2Cl3NO2	050995-94-3	60
5	3(2H)-Isoquinolinone, 1-amino-, ...	175	C9H9N3O	041536-79-2	59





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Quant Title : SW846 8260

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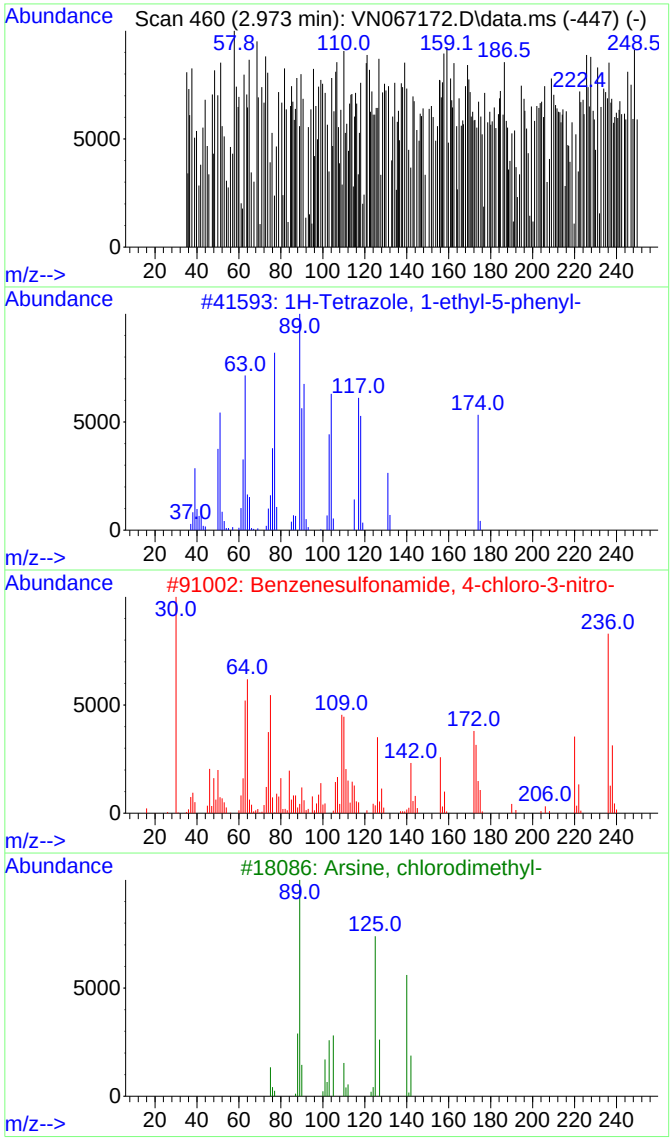
TIC Integration Parameters: LSCINT.P

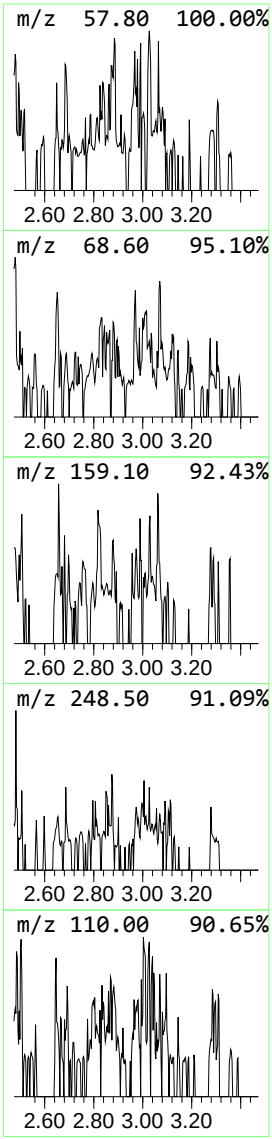
****

Peak Number 3 unknown2.973 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.973	6.04 ug/l	97735	Pentafluorobenzene	7.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Tetrazole, 1-ethyl-5-phenyl-	174	C9H10N4	024433-71-4	47
2	Benzenesulfonamide, 4-chloro-3-n...	236	C6H5ClN2O4S	000097-09-6	44
3	Arsine, chlorodimethyl-	140	C2H6AsCl	000557-89-1	43
4	4-Acetamido-3-nitrobenzoic acid	224	C9H8N2O5	001539-06-6	25
5	Benzene, 2-methoxy-1-methyl-3,5-...	212	C8H8N2O5	029027-13-2	25





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118-119

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

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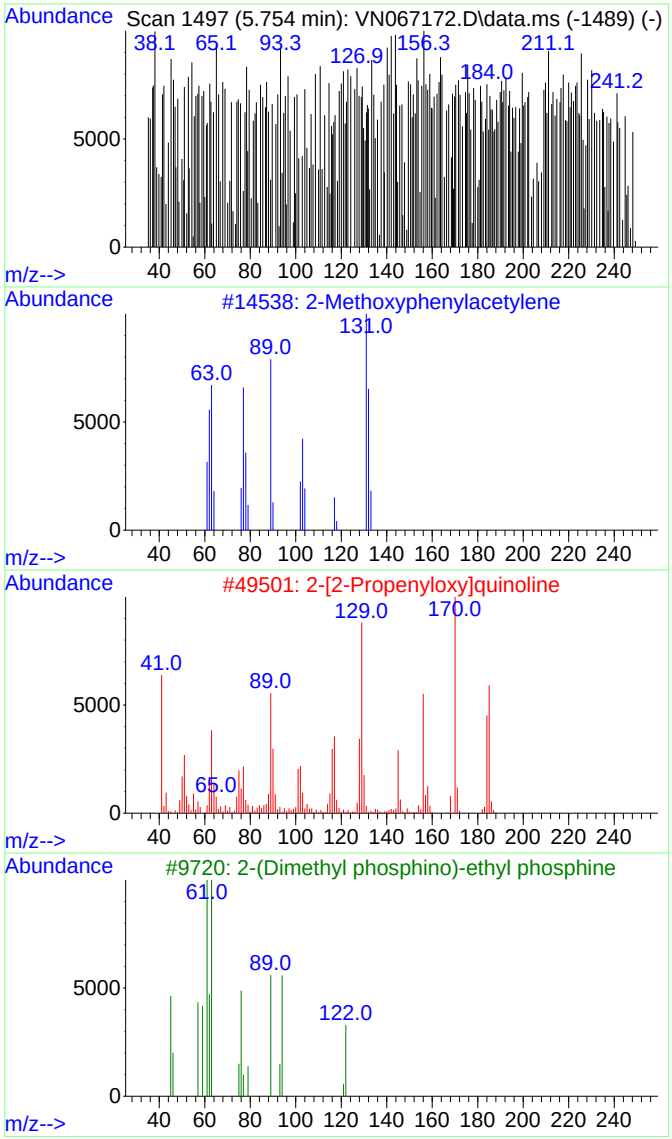
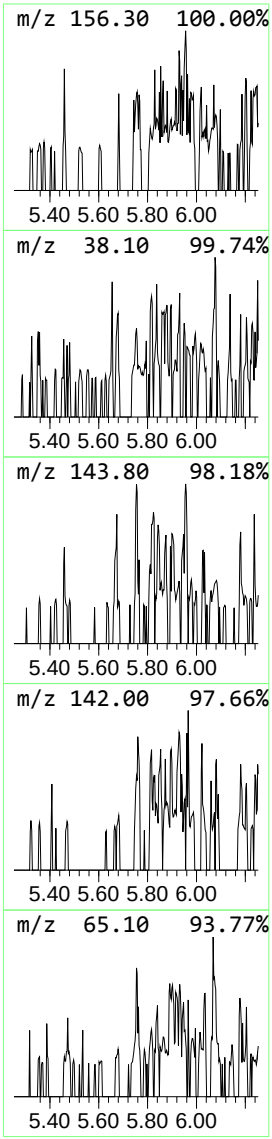
****
Peak Number 4 2-Methoxyphenylacetylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.754	5.39 ug/l	87296	Pentafluorobenzene	7.594

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxyphenylacetylene	132	C9H8O	000767-91-9	60
2	2-[2-Propenyloxy]quinoline	185	C12H11NO	000945-84-6	55
3	2-(Dimethyl phosphino)-ethyl pho...	122	C4H12P2	054772-64-4	49
4	Dicamba	220	C8H6Cl2O3	001918-00-9	46
5	4H-1-Benzopyran-4-one, 6-bromo-	224	C9H5BrO2	051483-92-2	46





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
6H-Indolo[3,2,1...	2.421	5.4	ug/l	88079	1	7.594	809392	50.0
s-Triazole-3-ca...	2.651	5.9	ug/l	95469	1	7.594	809392	50.0
unknown2.973	2.973	6.0	ug/l	97735	1	7.594	809392	50.0
2-Methoxyphenyl...	5.754	5.4	ug/l	87296	1	7.594	809392	50.0