

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074545.D
 Acq On : 17 Sep 2022 06:10
 Operator : JC\MD
 Sample : N4549-17
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-61

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\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074545.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	61	rBV	255234	490745	25.40%	4.302%
2	2.687	133	136	141	rBV2	48691	109423	5.66%	0.959%
3	2.728	141	143	154	rVB	78408	105809	5.48%	0.928%
4	3.169	216	218	229	rVB3	33528	73061	3.78%	0.640%
5	5.281	574	577	588	rVB5	12313	31025	1.61%	0.272%
6	5.528	608	619	620	rBV2	20093	40715	2.11%	0.357%
7	7.951	1019	1031	1036	rBV	265664	626914	32.45%	5.496%
8	8.016	1036	1042	1052	rVB	409526	929190	48.09%	8.145%
9	8.369	1091	1102	1115	rBV	298340	700442	36.25%	6.140%
10	8.904	1183	1193	1204	rBV	676932	1382510	71.55%	12.119%
11	10.380	1436	1444	1457	rBV	1056995	1932123	100.00%	16.937%
12	11.686	1656	1666	1676	rBV	1063784	1854759	96.00%	16.259%
13	12.521	1803	1808	1814	rVB4	14738	21866	1.13%	0.192%
14	12.674	1827	1834	1844	rBV	851982	1400256	72.47%	12.275%
15	13.615	1986	1994	2005	rBV	1056373	1683799	87.15%	14.760%
16	14.268	2100	2105	2112	rVB6	14925	24856	1.29%	0.218%

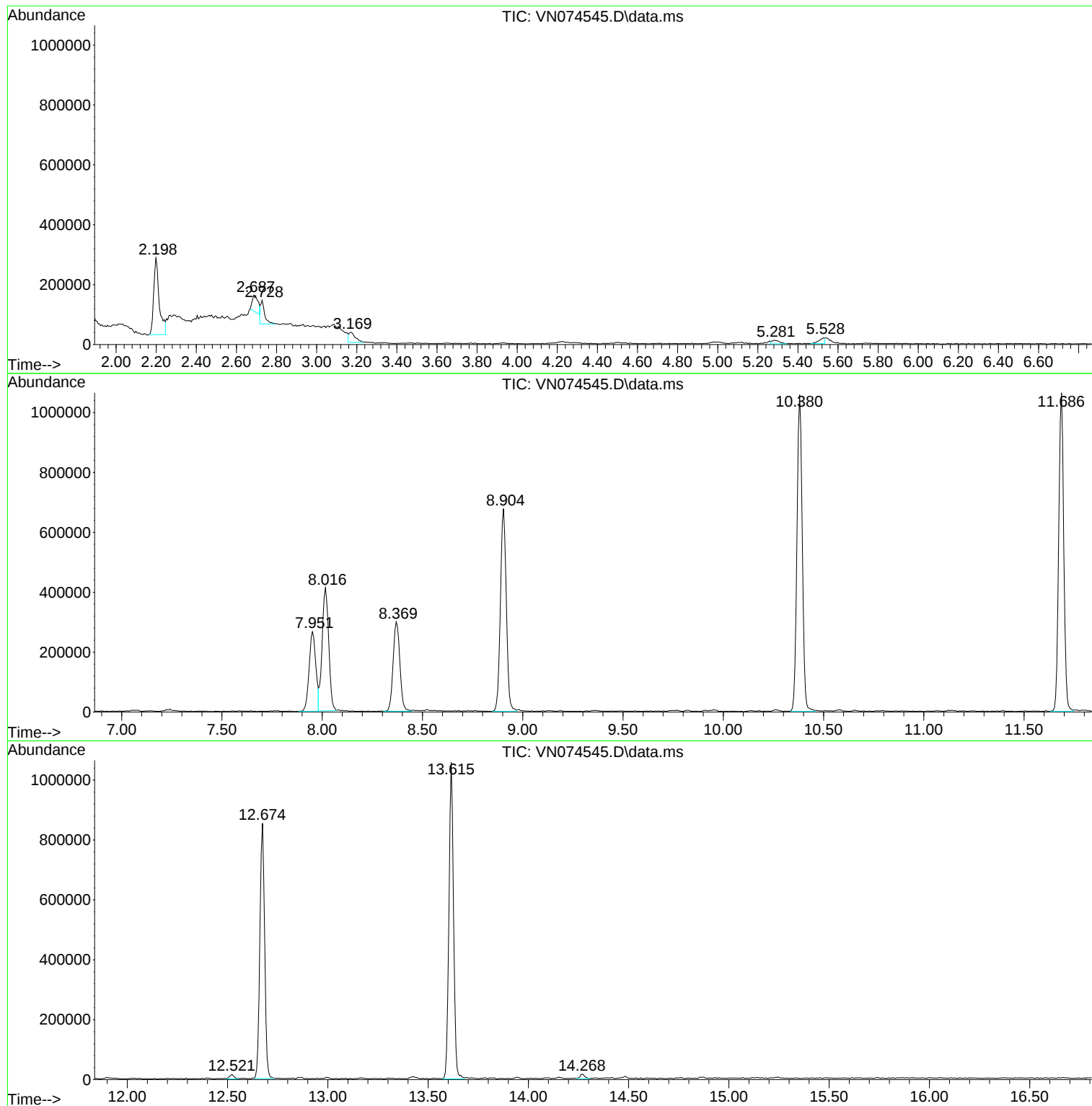
Sum of corrected areas: 11407493

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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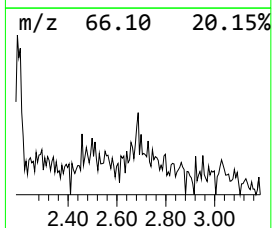
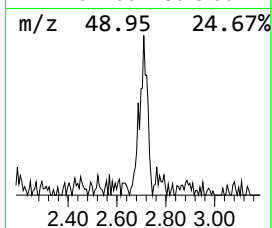
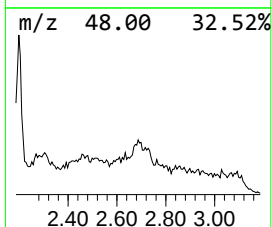
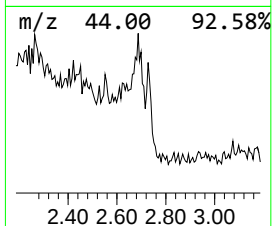
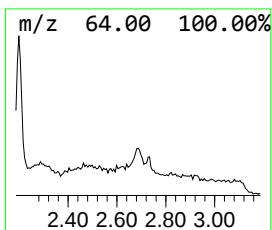
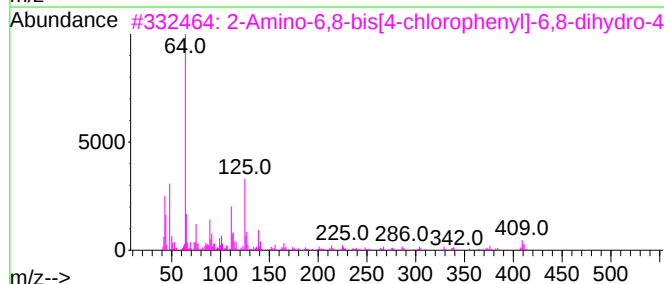
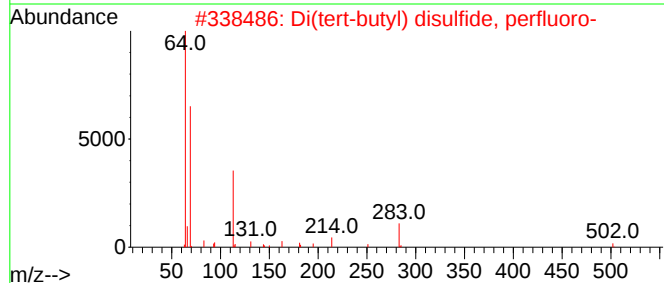
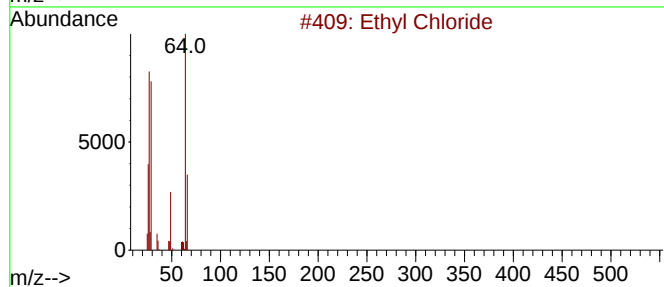
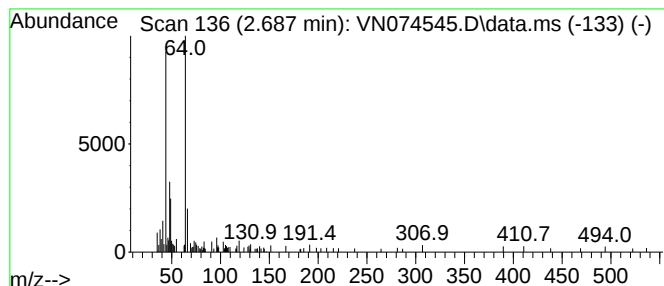
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.687 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
2.687	5.89 ug/l	109423	Pentafluorobenzene			8.016
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Ethyl Chloride		64	C2H5Cl	000075-00-3	42
2	Di(tert-butyl) disulfide, perflu...		502	C8F18S2	034880-30-3	39
3	2-Amino-6,8-bis[4-chlorophenyl]-...		473	C20H13Cl2N5O3S	049647-41-8	37
4	2-Sulfamyl-4,4'-diformamidodiphe...		383	C14H13N3O6S2	1000256-33-9	33
5	2,4,6-Triamino-5-pyrimidinyl hyd...		221	C4H7N5O4S	071552-23-3	28



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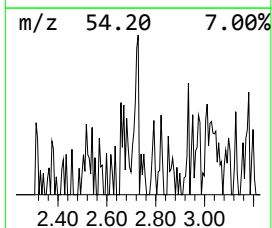
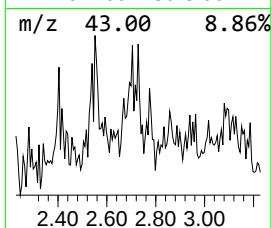
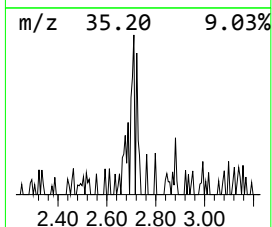
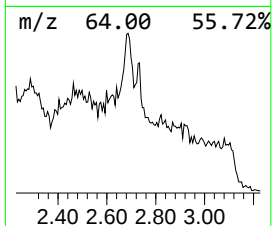
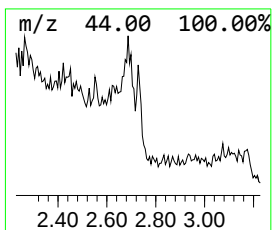
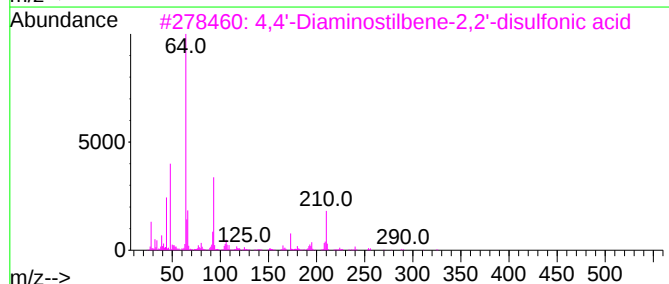
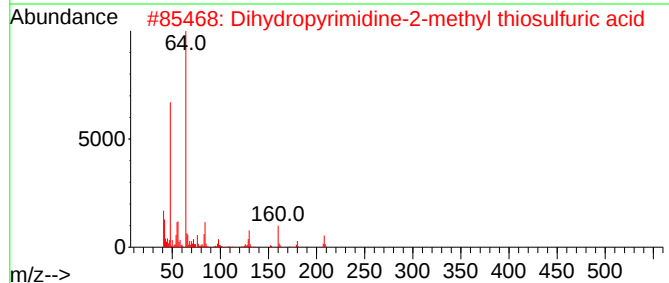
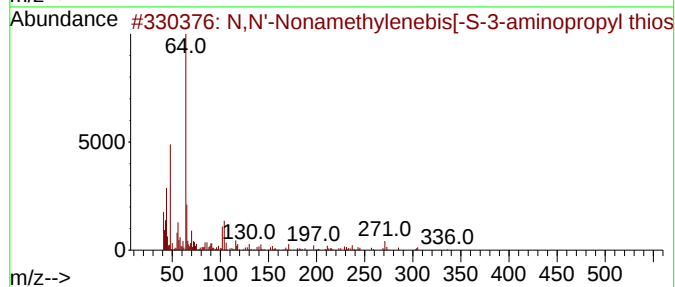
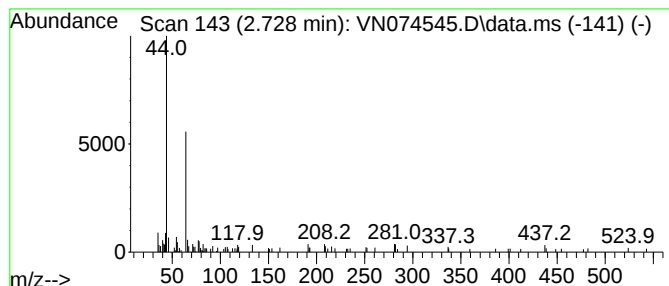
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Peak Number 3 unknown2.728 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.728	5.69 ug/l	105809	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	33
2			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	28
3			4,4'-Diaminostilbene-2,2'-disulf...	370	C14H14N2O6S2	000081-11-8	28
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	9
5			S-Methyl n-propylphosphonamidoth...	153	C4H12NOPS	1000306-04-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.687	2.687	5.9	ug/l	109423	1	8.016	929190	50.0
unknown2.728	2.728	5.7	ug/l	105809	1	8.016	929190	50.0