LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

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:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	4.952	311	317	325	rBV	323208	471718	3.67%	0.642%
2	5.416	388	396	406	rBV	6750912	9283992	72.28%	12.634%
3	7.004	657	666	682	rBV	6521547	9642253	75.07%	13.121%
4	7.840	800	808	817	rBV	1024326	1588997	12.37%	2.162%
5	8.993	995	1004	1014	rBV	3521203	5632113	43.85%	7.664%
6	10.634	1275	1283	1291	rBV	1180505	1982028	15.43%	2.697%
7	13.098	1694	1702	1711	rBV	8283697	11248689	87.57%	15.307%
8	14.469	1927	1935	1945	rBV	1418823	2082518	16.21%	2.834%
9	14.904	2000	2009	2018	rBV	136070	342607	2.67%	0.466%
10	15.827	2160	2166	2176	rBV	447332	620753	4.83%	0.845%
11	15.916	2176	2181	2182	rVV	201470	225631	1.76%	0.307%
12	15.951	2182	2187	2203	rVB	4895169	6541043	50.92%	8.901%
13	16.480	2271	2277	2284	rBV	350131	491564	3.83%	0.669%
14	16.551	2284	2289	2294	rVV	655014	833718	6.49%	1.135%
15	16.610	2294	2299	2304	rVV	740848	976375	7.60%	1.329%
16	16.668	2304	2309	2312	rVV	873576	1098219	8.55%	1.494%
17	16.710	2312	2316	2323	rVB	907086	1133782	8.83%	1.543%
18	17.204	2392	2400	2410	rBV	1531993	2102819	16.37%	2.862%
19	17.915	2515	2521	2531	rBV	427935	544375	4.24%	0.741%
20	19.821	2839	2845	2854	rBV	11675329	12845087	100.00%	17.480%
21	21.427	3113	3118	3127	rBV2	1238892	1838333	14.31%	2.502%
22	24.450	3624	3632	3650	rVB	808742	1959739	15.26%	2.667%

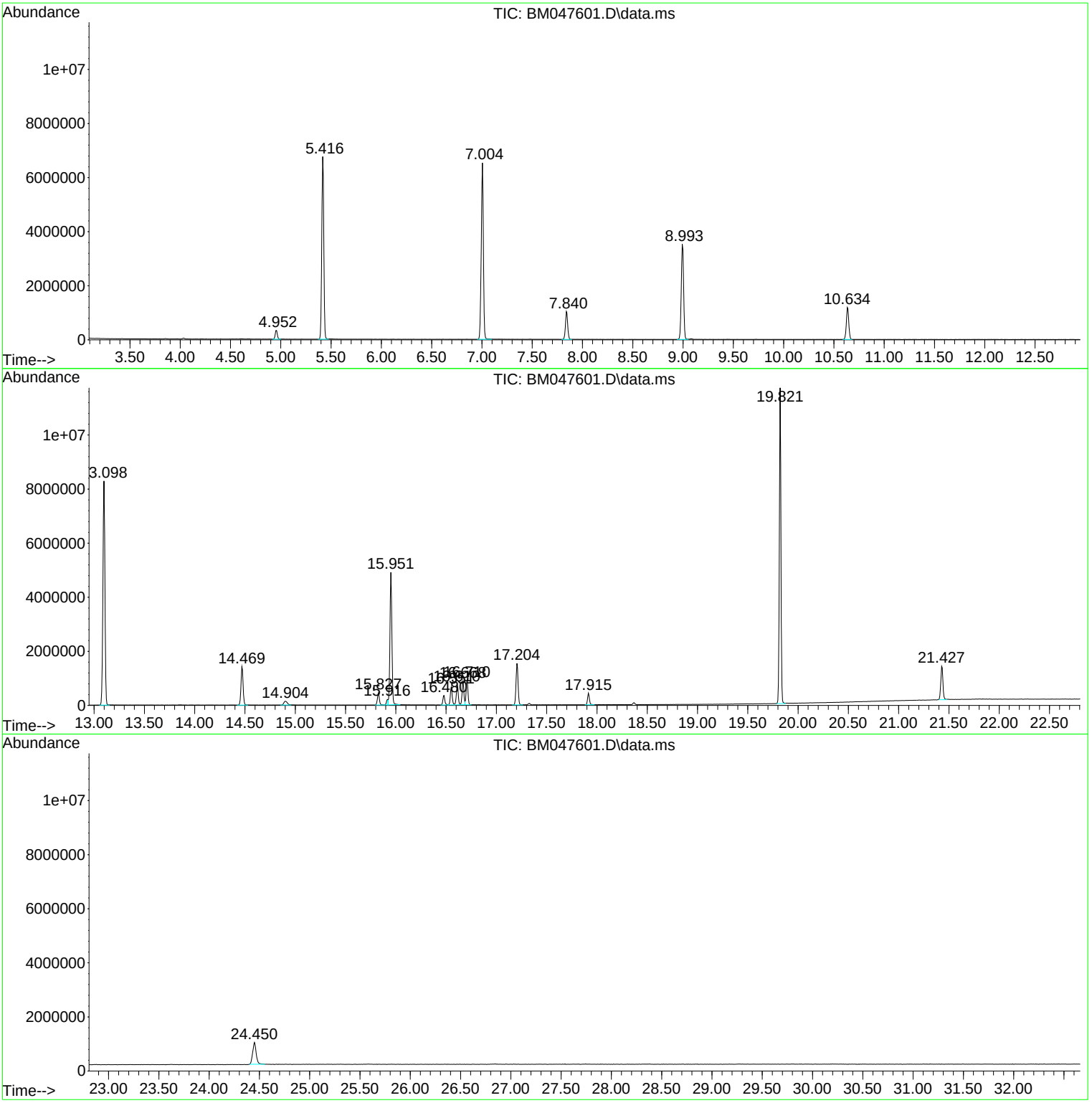
Sum of corrected areas: 73486353

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

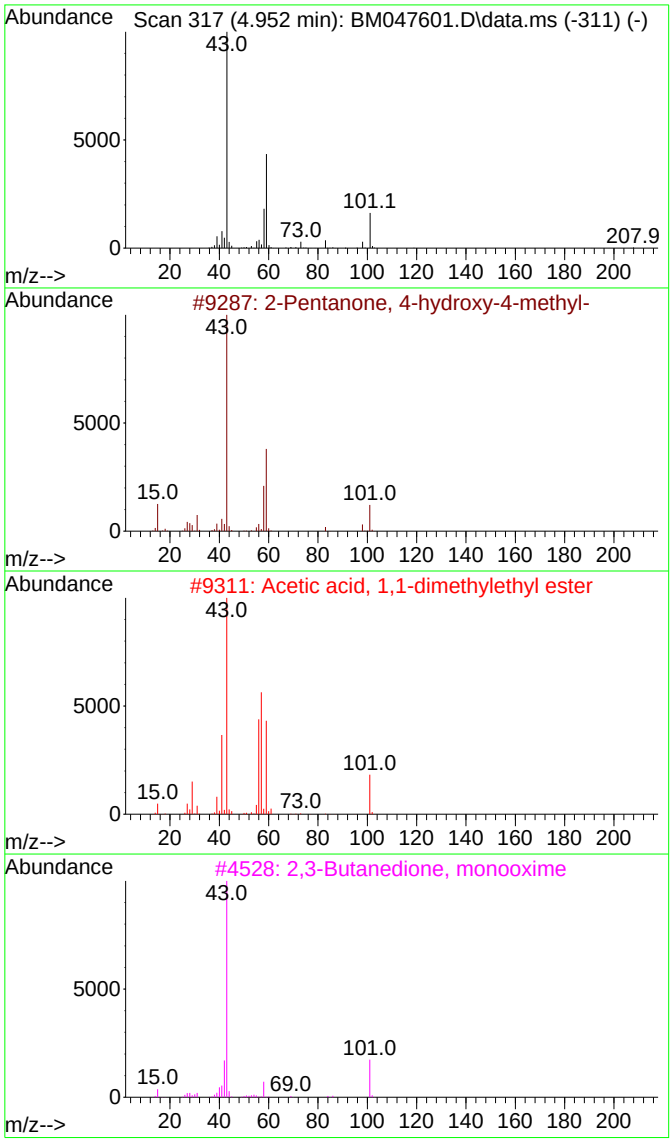
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

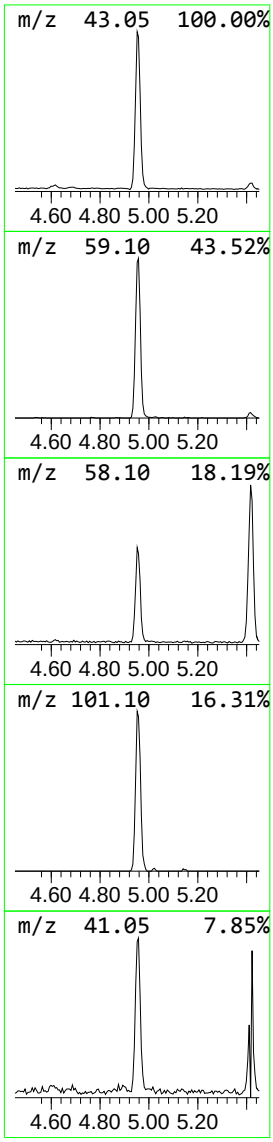
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	5.94 ng	471718	1,4-Dichlorobenzene-d4	7.840

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

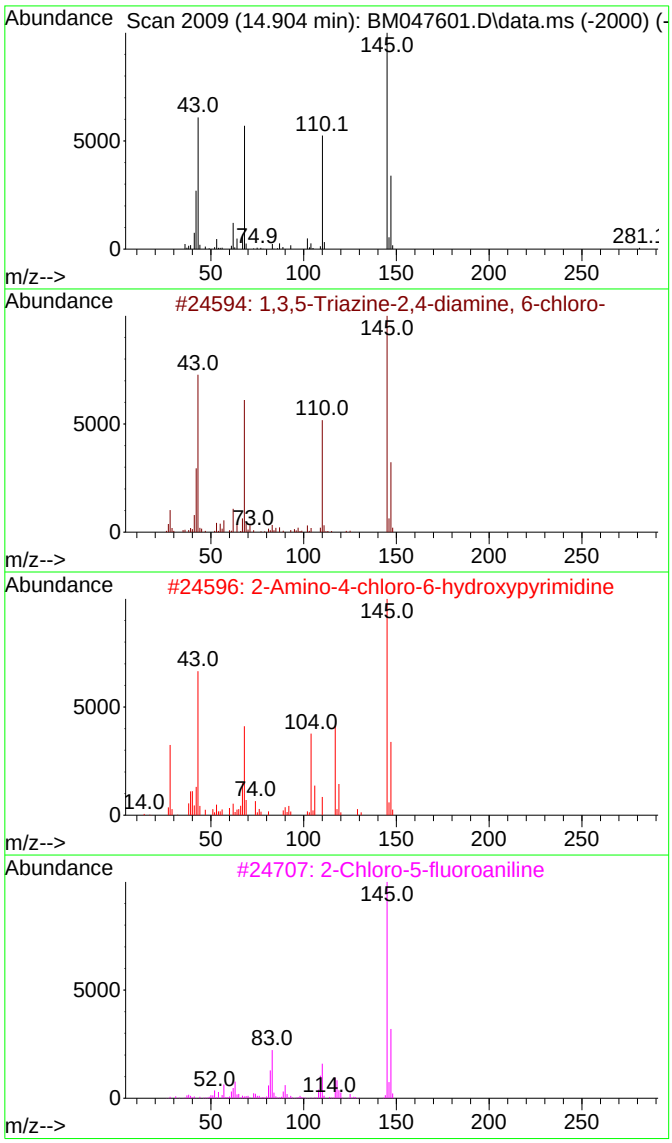
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

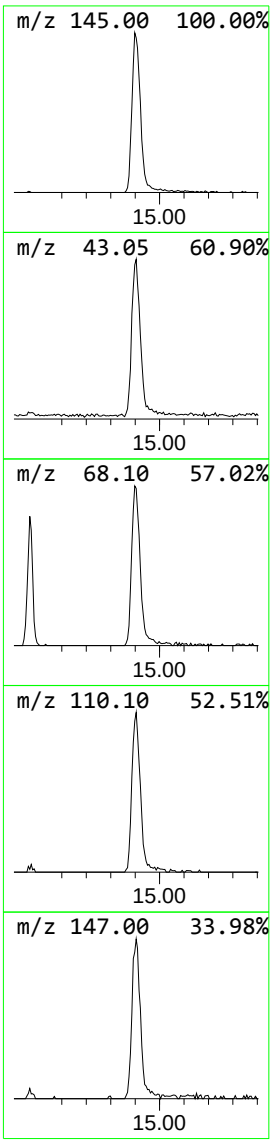
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,3,5-Triazine-2,4-diamine,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.29 ng	342607	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4-diamine, 6-ch...	145	C3H4ClN5	003397-62-4	95
2	2-Amino-4-chloro-6-hydroxypyrimi...	145	C4H4ClN3O	001194-21-4	42
3	2-Chloro-5-fluoroaniline	145	C6H5ClFN	000452-83-5	25
4	2-Chloro-4-fluoroaniline	145	C6H5ClFN	002106-02-7	25
5	2(1H)-Pyridinone, 5-chloro-3-hyd...	145	C5H4ClNO2	053233-89-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

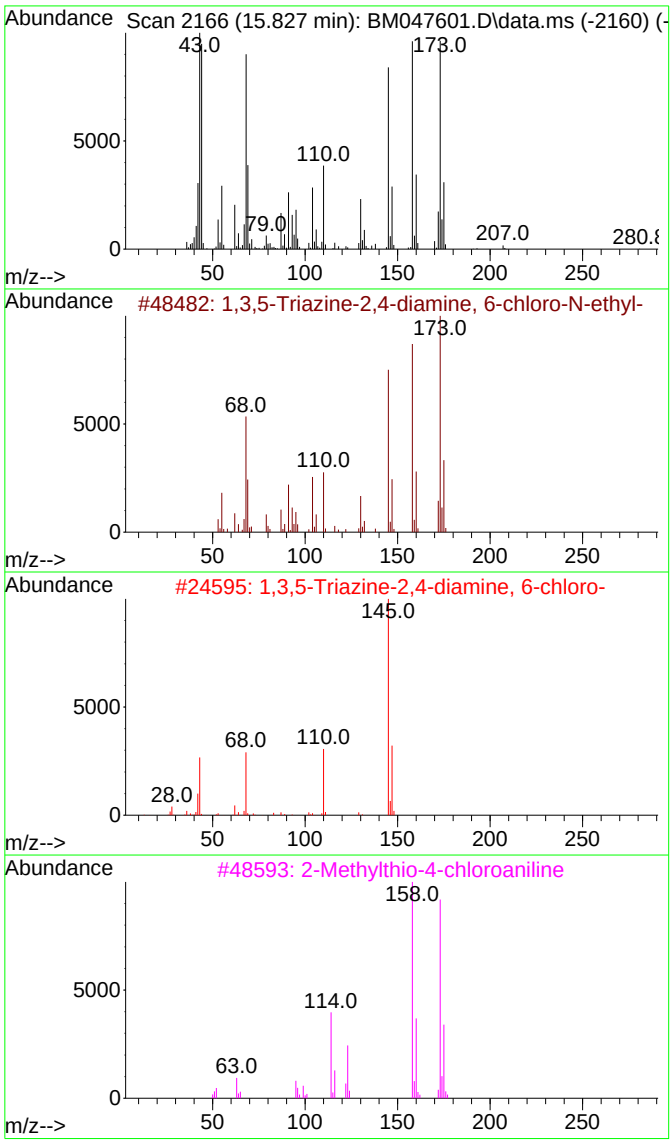
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

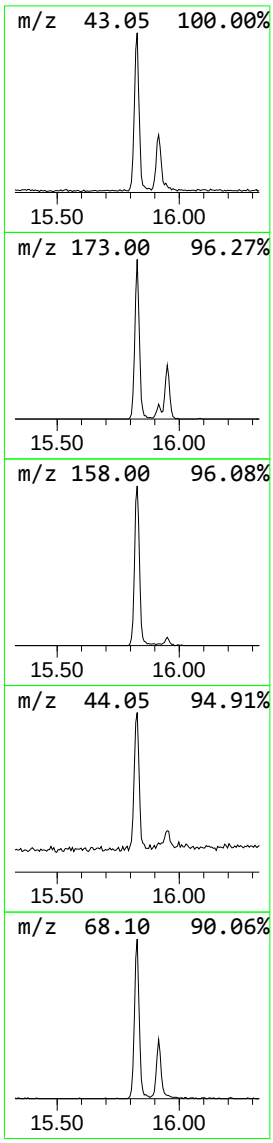
****

Peak Number 3 unknown15.827 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	5.96 ng	620753	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4-diamine, 6-ch...	173	C5H8ClN5	001007-28-9	98
2	1,3,5-Triazine-2,4-diamine, 6-ch...	145	C3H4ClN5	003397-62-4	30
3	2-Methylthio-4-chloroaniline	173	C7H8ClNS	029690-21-9	30
4	4-Trifluoromethylbenzoic acid, c...	258	C13H13F3O2	1000280-03-5	27
5	5-Pyrimidinamine, 2-chloro-4-eth...	173	C6H8ClN3O	054484-70-7	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

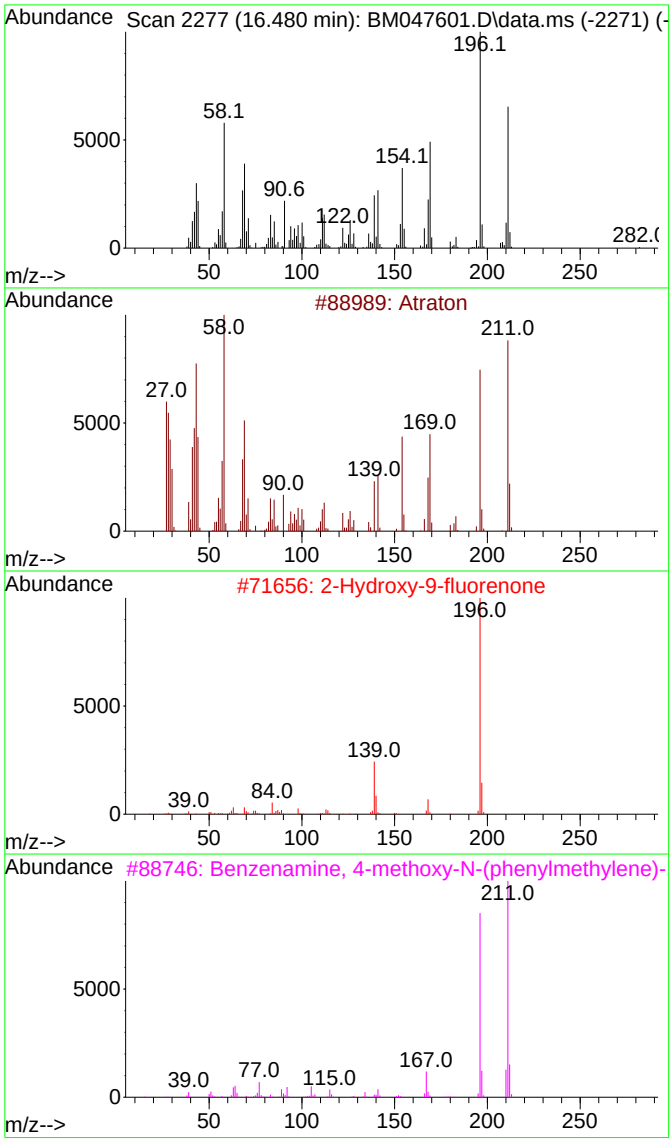
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

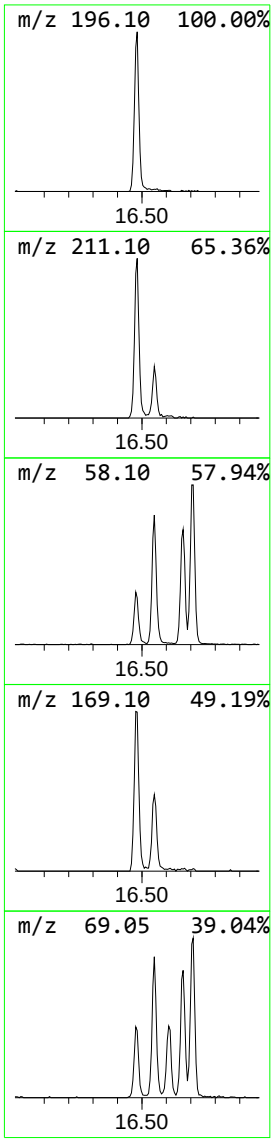
****

Peak Number 4 Atraton Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	4.68 ng	491564	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Atraton	211	C9H17N5O	001610-17-9	89
2	2-Hydroxy-9-fluorenone	196	C13H8O2	006949-73-1	35
3	Benzenamine, 4-methoxy-N-(phenyl...	211	C14H13NO	000783-08-4	35
4	1-[2-(Methylthio)-5-nitrophenyl]...	211	C9H9NO3S	1000266-40-0	25
5	N-(4-Acetylphenyl)-2-chloroaceta...	211	C10H10ClNO2	038283-38-4	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

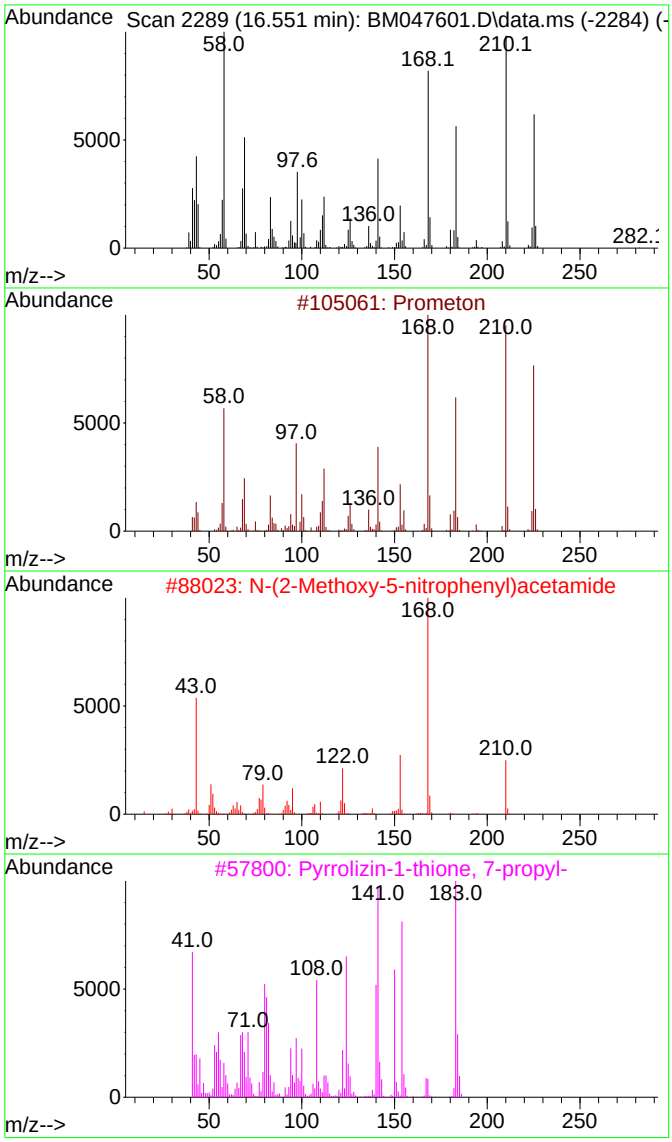
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

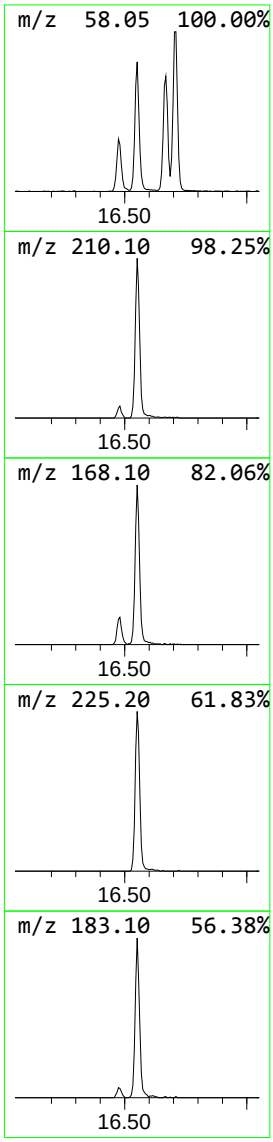
****

Peak Number 5 Prometon Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	7.93 ng	833718	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prometon	225	C10H19N5O	001610-18-0	99
2	N-(2-Methoxy-5-nitrophenyl)aceta...	210	C9H10N2O4	033721-54-9	25
3	Pyrrolizin-1-thione, 7-propyl-	183	C10H17NS	1000125-99-7	25
4	4-(2-Chlorophenyl)-1,3-thiazol-2...	210	C9H7ClN2S	021344-90-1	22
5	2-Methoxy-1-phenazinamine	225	C13H11N3O	003224-52-0	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

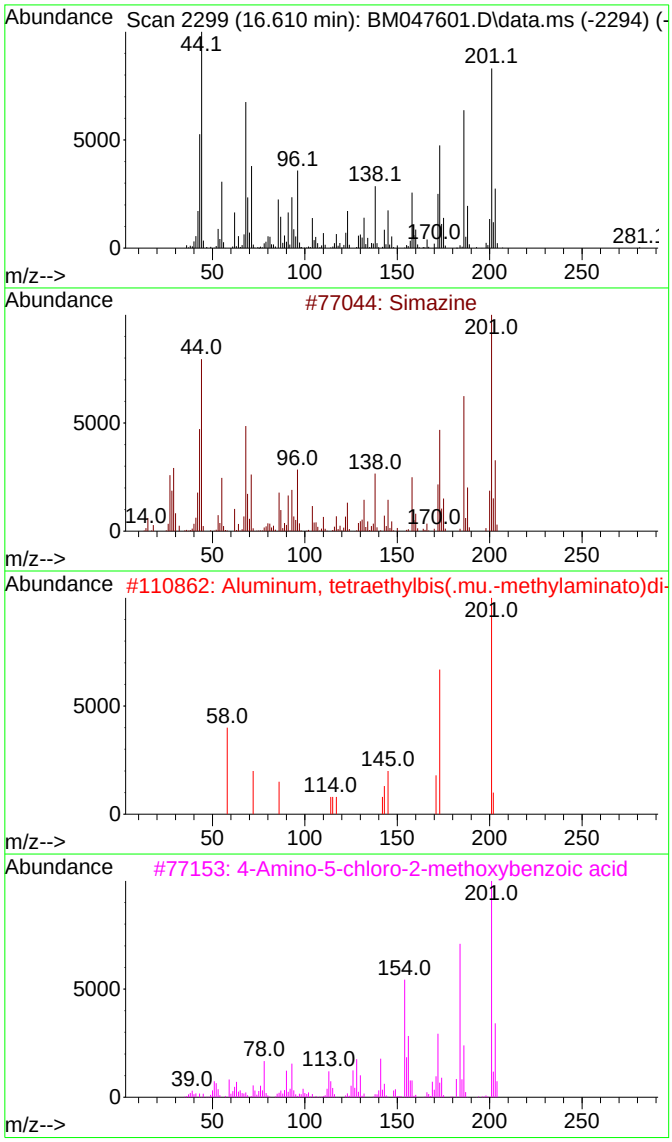
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

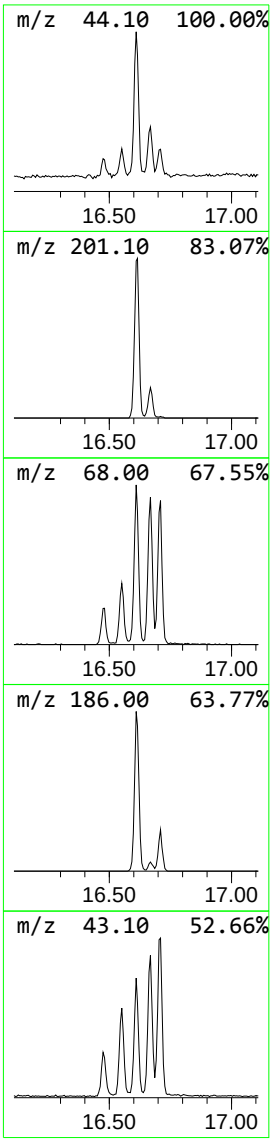
****

Peak Number 6 Simazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.610	9.29 ng	976375	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Simazine	201	C7H12ClN5	000122-34-9	99
2	Aluminum, tetraethylbis(.mu.-met...	230	C10H28Al2N2	023129-28-4	27
3	4-Amino-5-chloro-2-methoxybenzoi...	201	C8H8ClNO3	007206-70-4	25
4	3-Cyano-8-methoxycoumarin	201	C11H7NO3	013229-91-9	22
5	2,7-Naphthiridin-1(2H)-one, 4,5-...	201	C11H11N3O	1000260-79-4	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

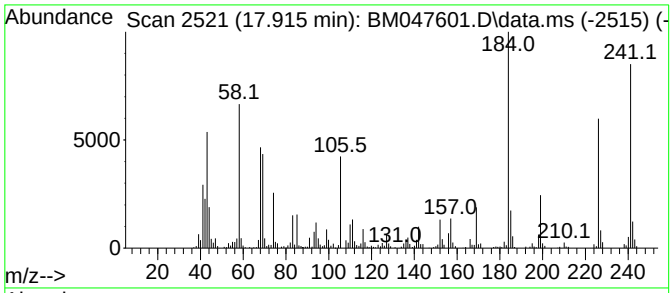
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

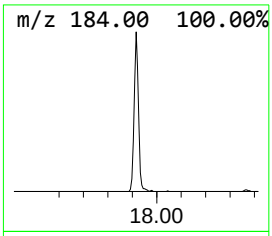
****

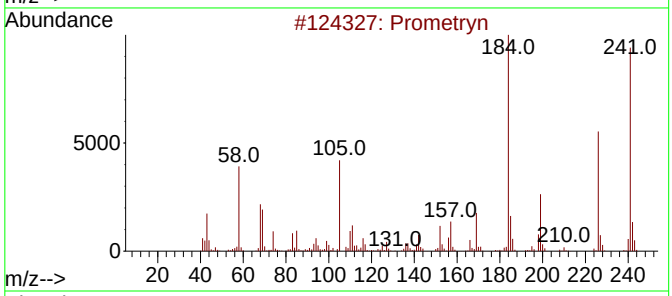
Peak Number 7 Prometryn Concentration Rank 5

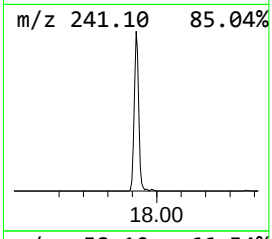
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.916	5.18 ng	544375	Phenanthrene-d10	17.204

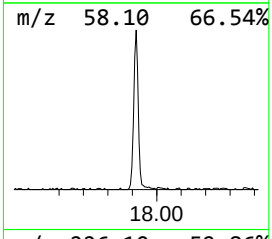
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prometryn	241	C10H19N5S	007287-19-6	99
2	N-(p-Methoxybenzylidene)-p-anisi...	241	C15H15NO2	001749-08-2	27
3	Thiazolo[5,4-d]pyrimidine, 6-ami...	226	C8H10N4S2	019844-40-7	25
4	Naphthalene, 1-[1-(S)-(dimethyla...	199	C14H17N	1010163-58-5	18
5	Benzenesulfonamide, 4-acetyl-	199	C8H9NO3S	001565-17-9	18

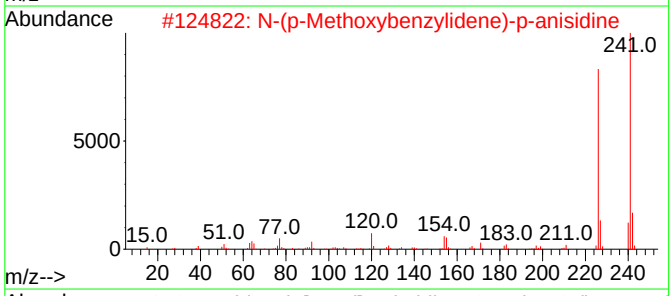


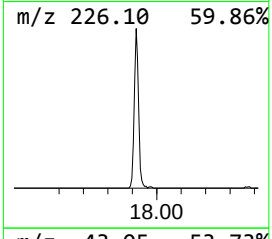


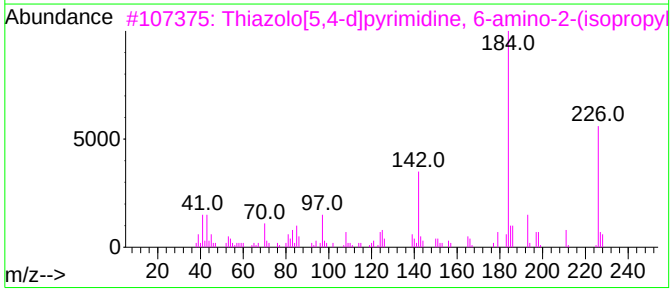


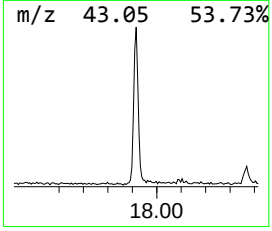












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
Data File : BM047601.D
Acq On : 23 Sep 2024 11:43
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.952	5.9	ng	471718	1	7.840	1589000	20.0
1,3,5-Triazine-...	14.904	3.3	ng	342607	3	14.469	2082520	20.0
unknown15.827	15.827	6.0	ng	620753	3	14.469	2082520	20.0
Atraton	16.480	4.7	ng	491564	4	17.204	2102820	20.0
Prometon	16.551	7.9	ng	833718	4	17.204	2102820	20.0
Simazine	16.610	9.3	ng	976375	4	17.204	2102820	20.0
Prometryn	17.916	5.2	ng	544375	4	17.204	2102820	20.0