LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
Data File : BM047570.D
Acq On : 19 Sep 2024 14:34
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 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-BM091424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.952	312	317	326	rBV	390172	553381	3.46%	0.627%
2	5.416	388	396	406	rBV	7557935	10508689	65.80%	11.913%
3	7.004	658	666	681	rBV	7135830	10869310	68.05%	12.322%
4	7.840	801	808	817	rVB	1183262	1843910	11.55%	2.090%
5	8.993	996	1004	1015	rBV	4166763	6605477	41.36%	7.488%
6	10.634	1276	1283	1293	rBV	1388478	2334629	14.62%	2.647%
7	13.098	1694	1702	1712	rBV	9162135	12847448	80.44%	14.564%
8	14.469	1928	1935	1945	rBV	1716848	2506498	15.69%	2.841%
9	14.904	2001	2009	2022	rBV2	172715	457139	2.86%	0.518%
10	15.827	2159	2166	2173	rBV	591484	843418	5.28%	0.956%
11	15.916	2175	2181	2182	rVV	283685	317808	1.99%	0.360%
12	15.951	2182	2187	2205	rVB	6074552	8276094	51.82%	9.382%
13	16.474	2271	2276	2284	rBV	520209	714137	4.47%	0.810%
14	16.551	2284	2289	2294	rVV	928136	1172875	7.34%	1.330%
15	16.610	2294	2299	2304	rVV	991780	1314813	8.23%	1.491%
16	16.669	2304	2309	2312	rVV2	1168920	1458328	9.13%	1.653%
17	16.710	2312	2316	2328	rVB	1218046	1515396	9.49%	1.718%
18	17.204	2392	2400	2409	rBV	1893744	2620589	16.41%	2.971%
19	17.915	2516	2521	2527	rBV	642567	766626	4.80%	0.869%
20	19.821	2839	2845	2856	rBV	13761137	15971375	100.00%	18.106%
21	21.433	3113	3119	3125	rBV	1626282	2345114	14.68%	2.658%
22	24.456	3625	3633	3642	rBV	999106	2369753	14.84%	2.686%

Sum of corrected areas: 88212807

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
Data File : BM047570.D
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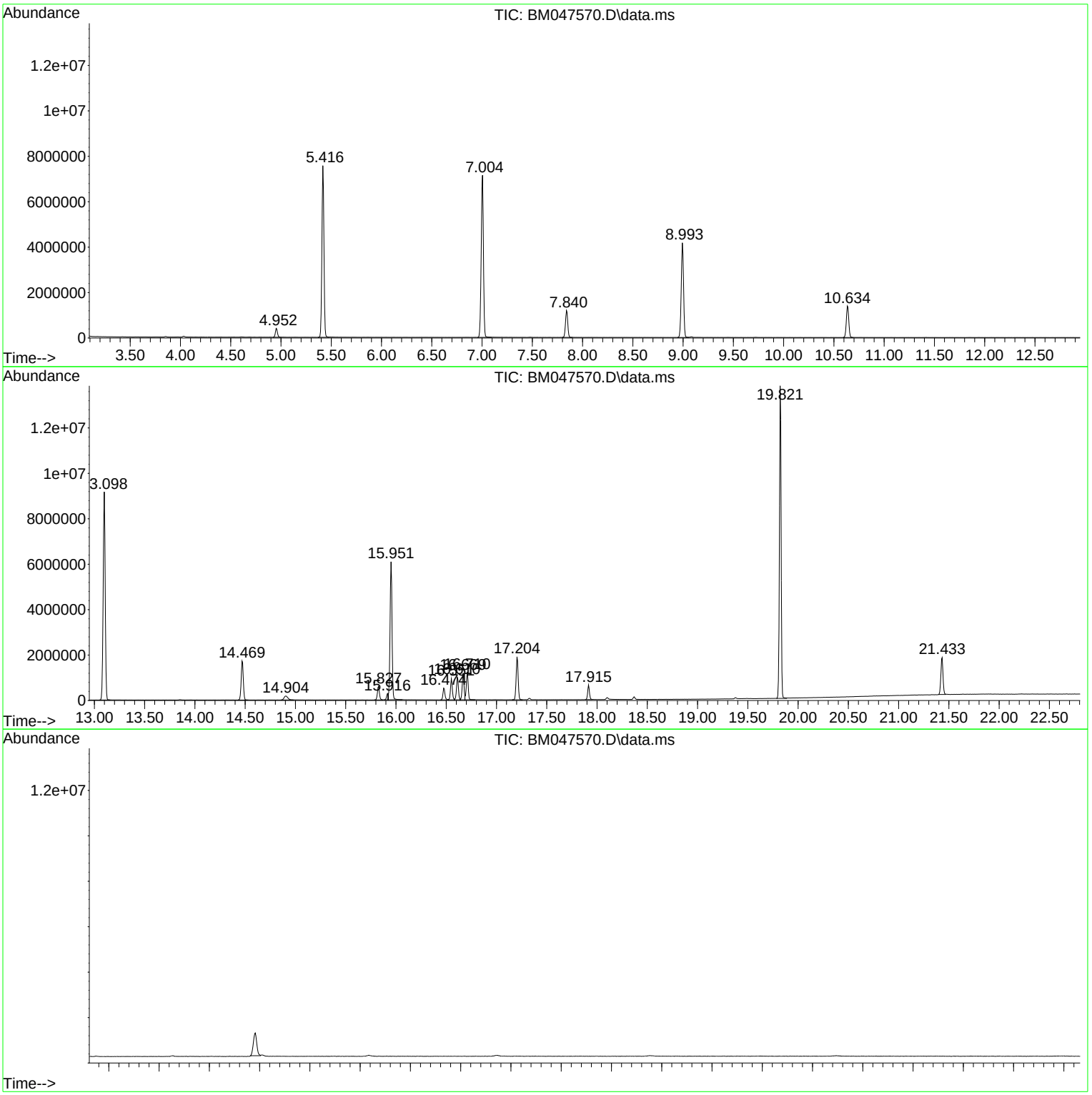
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.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\BM091924\
Data File : BM047570.D
Acq On : 19 Sep 2024 14:34
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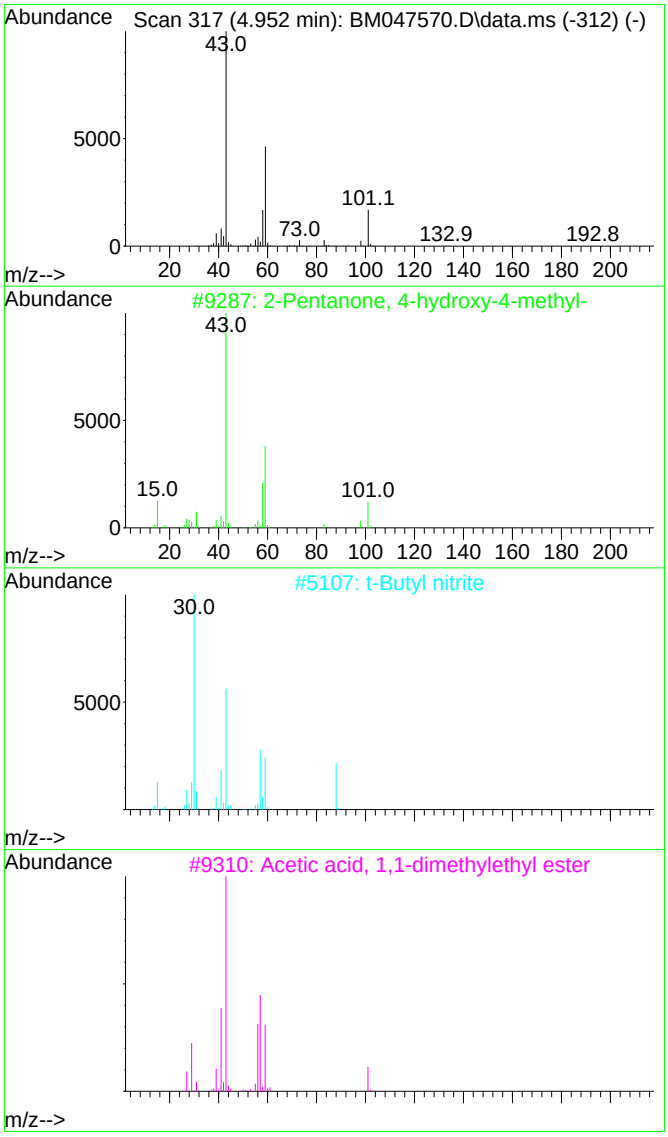
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

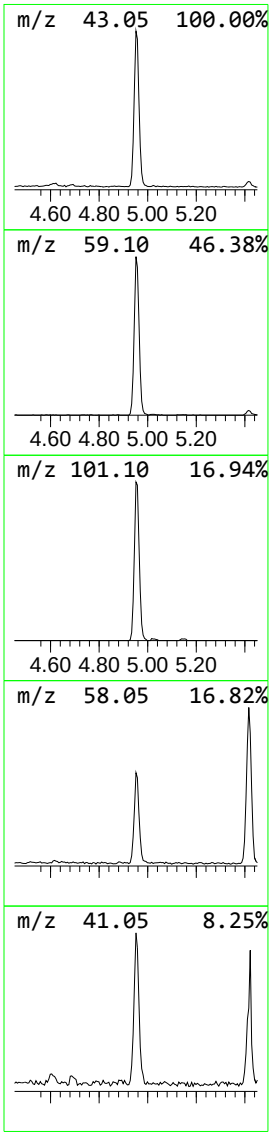
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.952	6.00 ng	553381	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	59
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	17
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
Data File : BM047570.D
Acq On : 19 Sep 2024 14:34
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

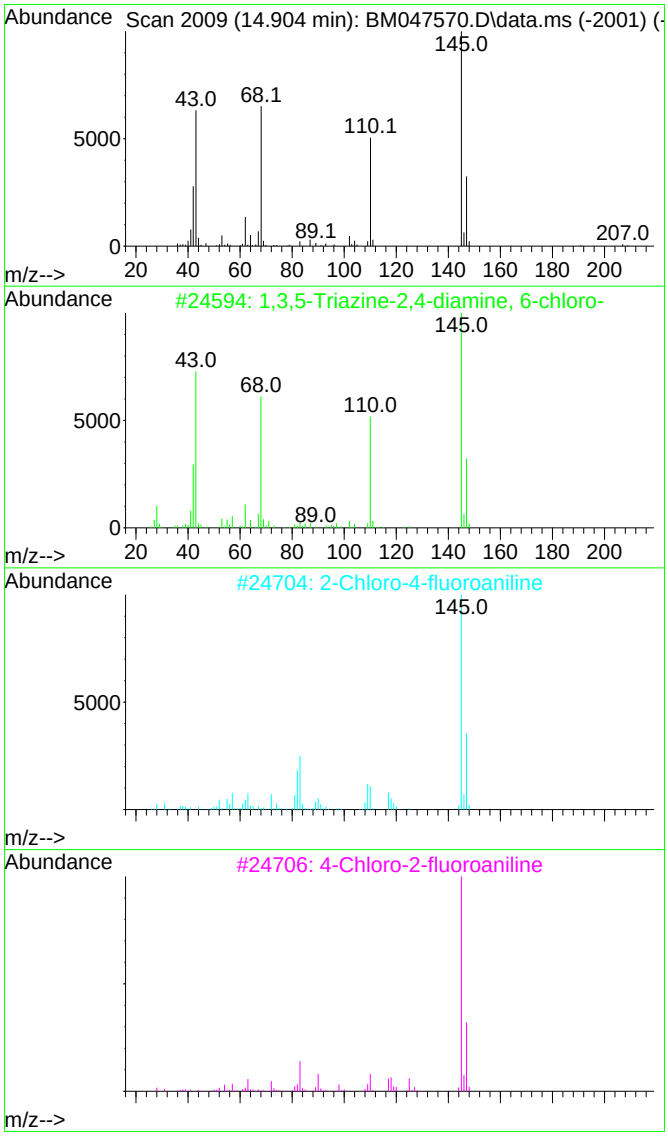
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

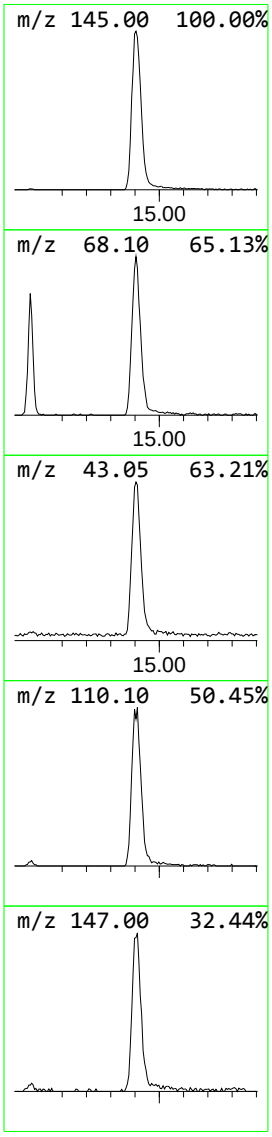
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	3.65 ng	457139	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	97
2	2-Chloro-4-fluoroaniline	145	C6H5ClFN	002106-02-7	30
3	4-Chloro-2-fluoroaniline	145	C6H5ClFN	057946-56-2	25
4	3-Chloropyridine-2-thiol, Ac der...	187	C7H6ClNOS	1000509-66-8	25
5	4-Chloro-3-fluoroaniline	145	C6H5ClFN	000367-22-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
Data File : BM047570.D
Acq On : 19 Sep 2024 14:34
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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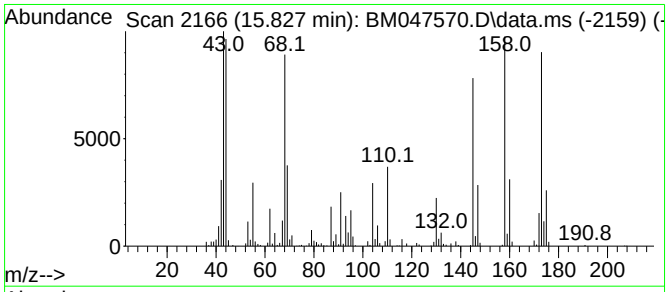
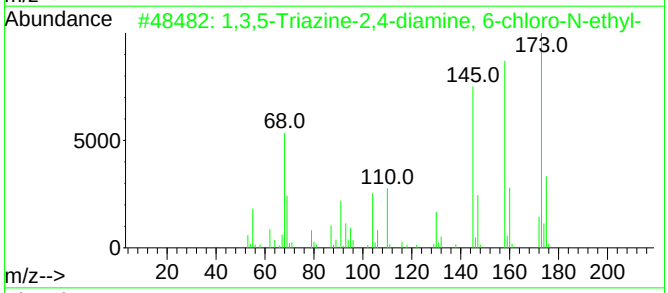
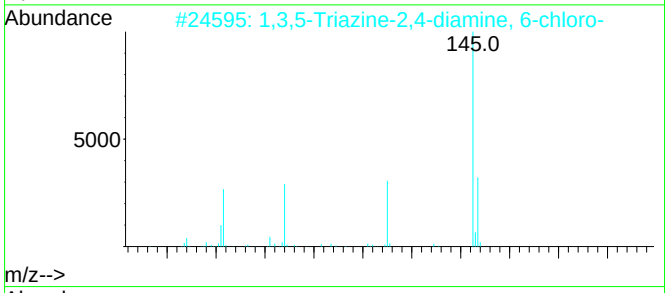
Peak Number 3 unknown15.827 Concentration Rank 3

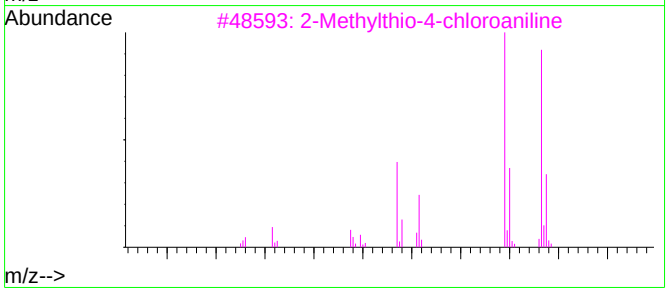
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.827	6.73 ng	843418	Acenaphthene-d10	14.469

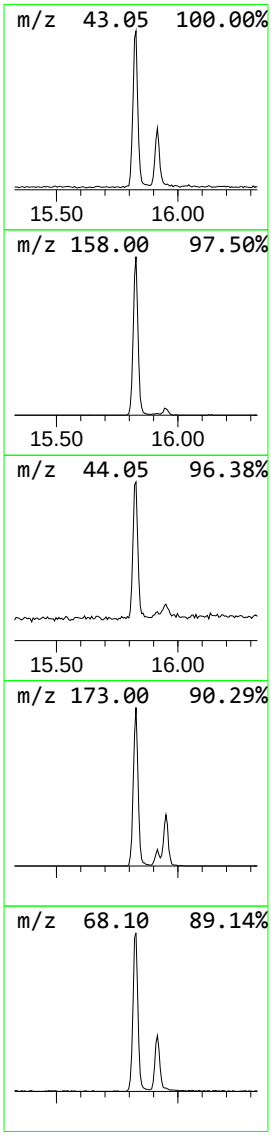
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4-diamine, 6-ch...	173	C5H8ClN5	001007-28-9	99
2	1,3,5-Triazine-2,4-diamine, 6-ch...	145	C3H4ClN5	003397-62-4	42
3	2-Methylthio-4-chloroaniline	173	C7H8ClNS	029690-21-9	38
4	4-Trifluoromethylbenzoic acid, c...	258	C13H13F3O2	1000280-03-5	35
5	2-Amino-4-chloro-6-hydroxypyrimi...	145	C4H4ClN3O	001194-21-4	30











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Data File : BM047570.D
Acq On : 19 Sep 2024 14:34
Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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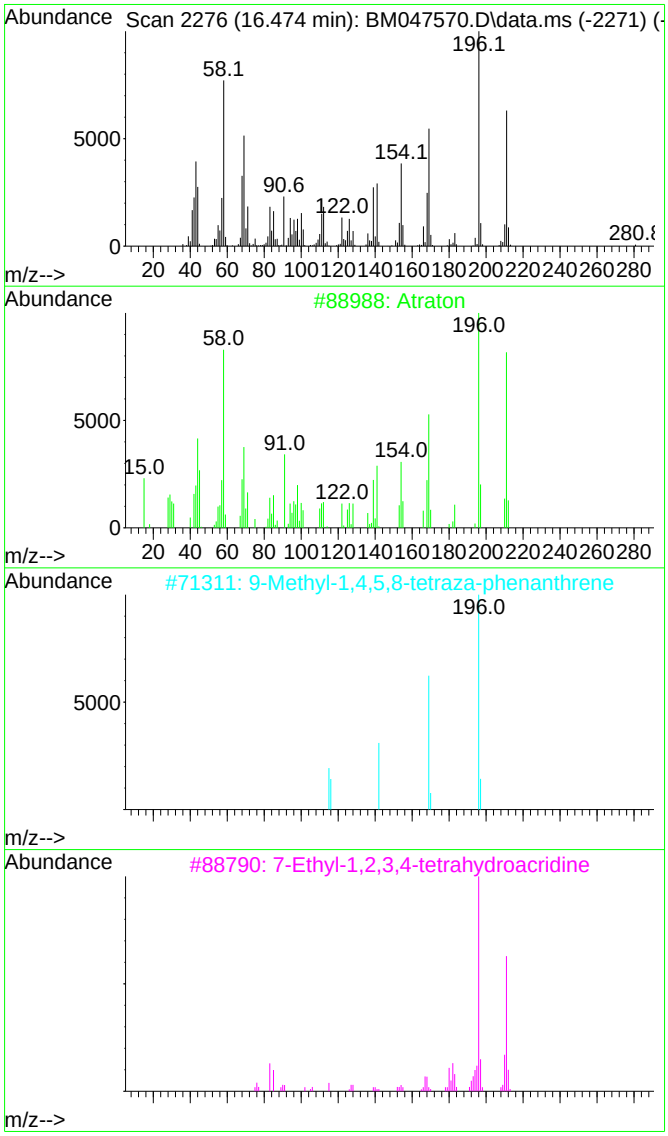
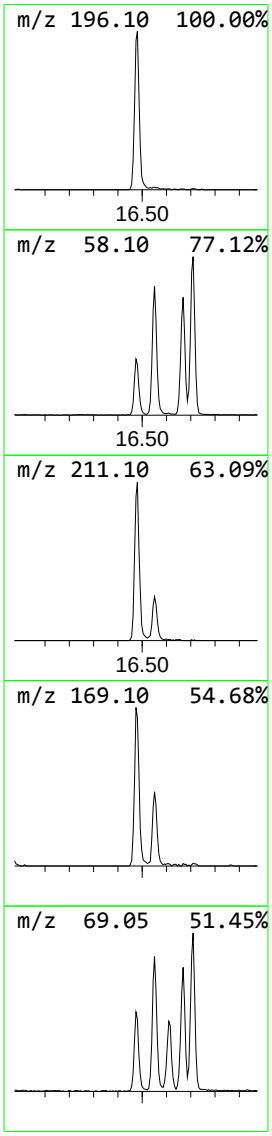
Peak Number 4 Atraton Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.474	5.45 ng	714137	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Atraton	211	C9H17N5O	001610-17-9	89
2	9-Methyl-1,4,5,8-tetraza-phenant...	196	C11H8N4	062088-23-7	35
3	7-Ethyl-1,2,3,4-tetrahydroacridine	211	C15H17N	055751-81-0	27
4	.beta.-Carboline, 1,2-dimethyl-	196	C13H12N2	109847-05-4	25
5	Thieno[2,3-b]thiophen-2-amine, N...	211	C10H13NS2	134662-66-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
Data File : BM047570.D
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Operator : RC/JU
Sample : P3845-22
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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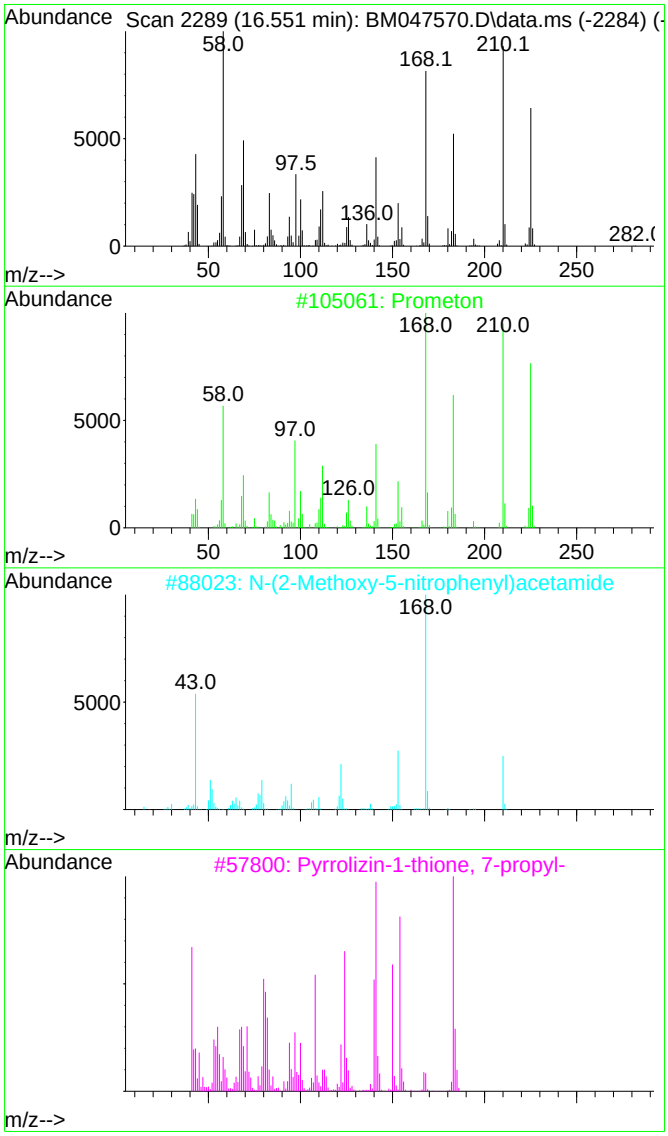
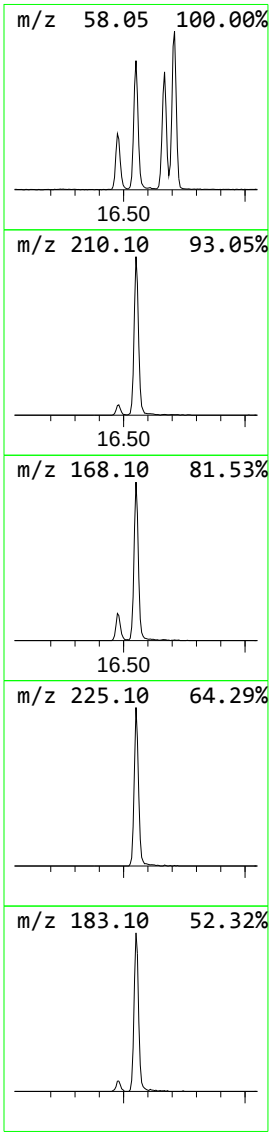
Peak Number 5 Prometon Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	8.95 ng	1172880	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	5-Acetamido-1,2,3-trimethoxybenzene	225	C11H15NO4	004304-24-9	14
5	2-Methoxy-1-phenazinamine	225	C13H11N3O	003224-52-0	14





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ClientSampleId :
RR-TRIAZINE-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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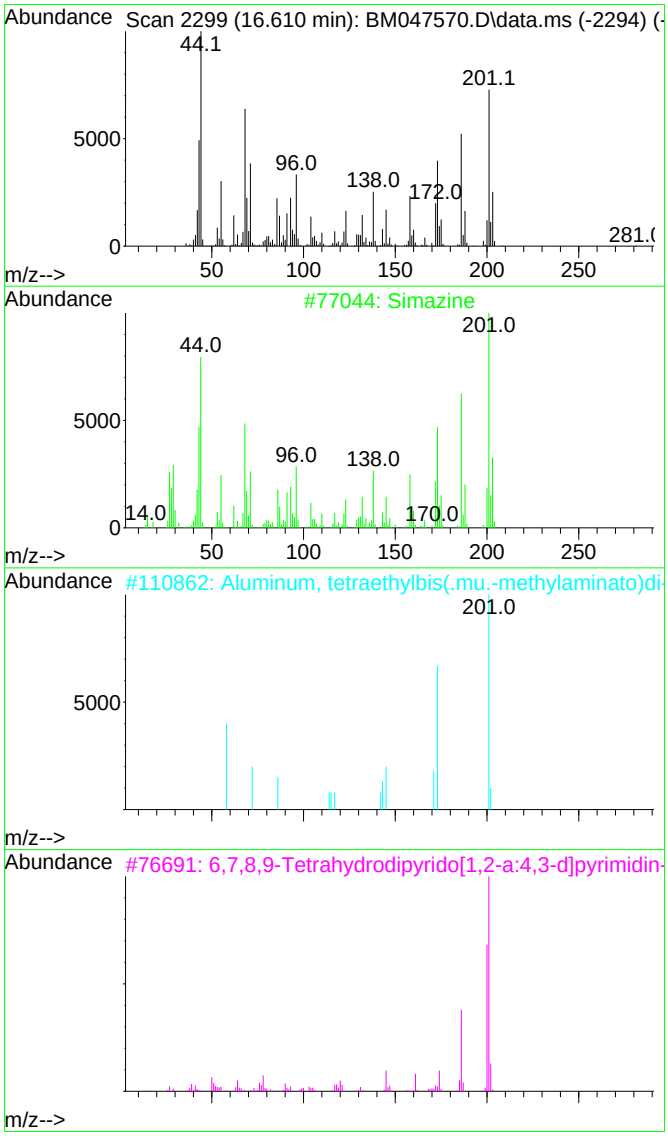
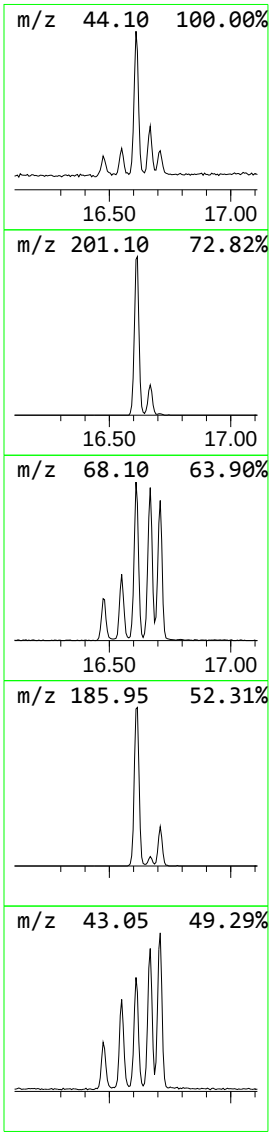
Peak Number 6 Simazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.610	10.03 ng	1314810	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	14
3	6,7,8,9-Tetrahydrodipyrido[1,2-a...	201	C11H11N3O	148056-89-7	11
4	2,5-Dimethyl-1-[(2-hydroxymethyl...	201	C13H15NO	097690-10-3	11
5	Furo[3,2-c]quinoline-2,4(3H,5H)-...	201	C11H7NO3	306320-38-7	11





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ALS Vial : 6 Sample Multiplier: 1

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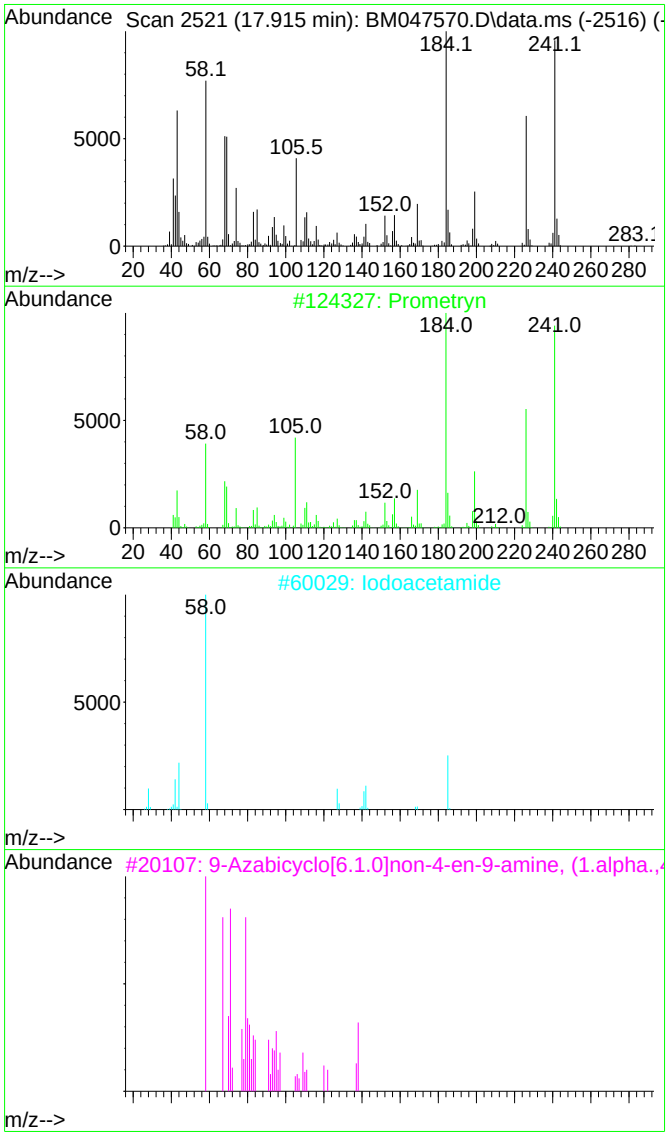
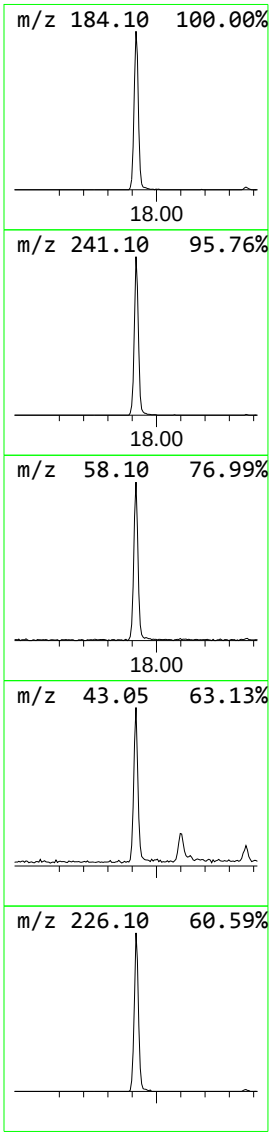
Peak Number 7 Prometryn Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.916	5.85 ng	766626	Phenanthrene-d10	17.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Prometryn	241	C10H19N5S	007287-19-6	99
2	Iodoacetamide	185	C2H4INO	000144-48-9	25
3	9-Azabicyclo[6.1.0]non-4-en-9-am...	138	C8H14N2	066387-78-8	15
4	Dibenzothiophene	184	C12H8S	000132-65-0	11
5	1H-Pyrazole-5-carboxylic acid, 3...	241	C13H11N3O2	1000362-41-4	11





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.952	6.0	ng	553381	1	7.840	1843910	20.0
1,3,5-Triazine-...	14.904	3.6	ng	457139	3	14.469	2506500	20.0
unknown15.827	15.827	6.7	ng	843418	3	14.469	2506500	20.0
Atraton	16.474	5.5	ng	714137	4	17.204	2620590	20.0
Prometon	16.551	8.9	ng	1172880	4	17.204	2620590	20.0
Simazine	16.610	10.0	ng	1314810	4	17.204	2620590	20.0
Prometryn	17.916	5.8	ng	766626	4	17.204	2620590	20.0