LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070218\
Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

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_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.190	482	485	496	rBV	62326	71670	4.01%	0.587%
2	5.601	552	555	572	rBV	766810	722405	40.37%	5.914%
3	6.601	722	725	736	rBV	459542	492838	27.54%	4.035%
4	6.737	744	748	751	rBV	1381835	1215851	67.95%	9.953%
5	6.954	782	785	789	rBV	407901	338610	18.92%	2.772%
6	7.113	808	812	815	rBV	1349217	1204883	67.33%	9.864%
7	7.525	877	882	885	rBV	979796	907355	50.71%	7.428%
8	7.760	916	922	929	rBV	32405	35513	1.98%	0.291%
9	8.242	1000	1004	1015	rBV	379476	386493	21.60%	3.164%
10	9.313	1182	1186	1189	rBV	1771141	1586440	88.66%	12.987%
11	9.648	1241	1243	1249	rVB	28356	19176	1.07%	0.157%
12	9.707	1249	1253	1259	rBV	82997	81778	4.57%	0.669%
13	10.001	1299	1303	1313	rVB	422252	388156	21.69%	3.178%
14	10.795	1434	1438	1446	rBV	963483	921399	51.49%	7.543%
15	10.860	1446	1449	1455	rVV2	20609	32391	1.81%	0.265%
16	10.907	1455	1457	1463	rVV	53025	44596	2.49%	0.365%
17	10.960	1463	1466	1468	rVV	133372	99570	5.56%	0.815%
18	10.989	1468	1471	1475	rVV2	103246	137895	7.71%	1.129%
19	11.025	1475	1477	1480	rVV	137915	128575	7.19%	1.053%
20	11.054	1480	1482	1484	rVV	77486	60303	3.37%	0.494%
21	11.095	1484	1489	1490	rVV	57560	66413	3.71%	0.544%
22	11.107	1490	1491	1493	rVV	53320	37957	2.12%	0.311%
23	11.142	1493	1497	1500	rVV3	123953	138299	7.73%	1.132%
24	11.177	1500	1503	1505	rVV	149292	118804	6.64%	0.973%
25	11.219	1508	1510	1513	rVB	82973	64259	3.59%	0.526%
26	11.377	1533	1537	1541	rBV3	25170	25862	1.45%	0.212%
27	11.495	1553	1557	1563	rVB	458993	390356	21.81%	3.196%
28	12.966	1804	1807	1814	rVB2	20324	28173	1.57%	0.231%
29	13.077	1822	1826	1829	rBV	1828949	1789430	100.00%	14.649%
30	14.148	2004	2008	2014	rBV	440391	399853	22.35%	3.273%
31	15.689	2265	2270	2278	rVB	207954	280103	15.65%	2.293%

Sum of corrected areas: 12215406

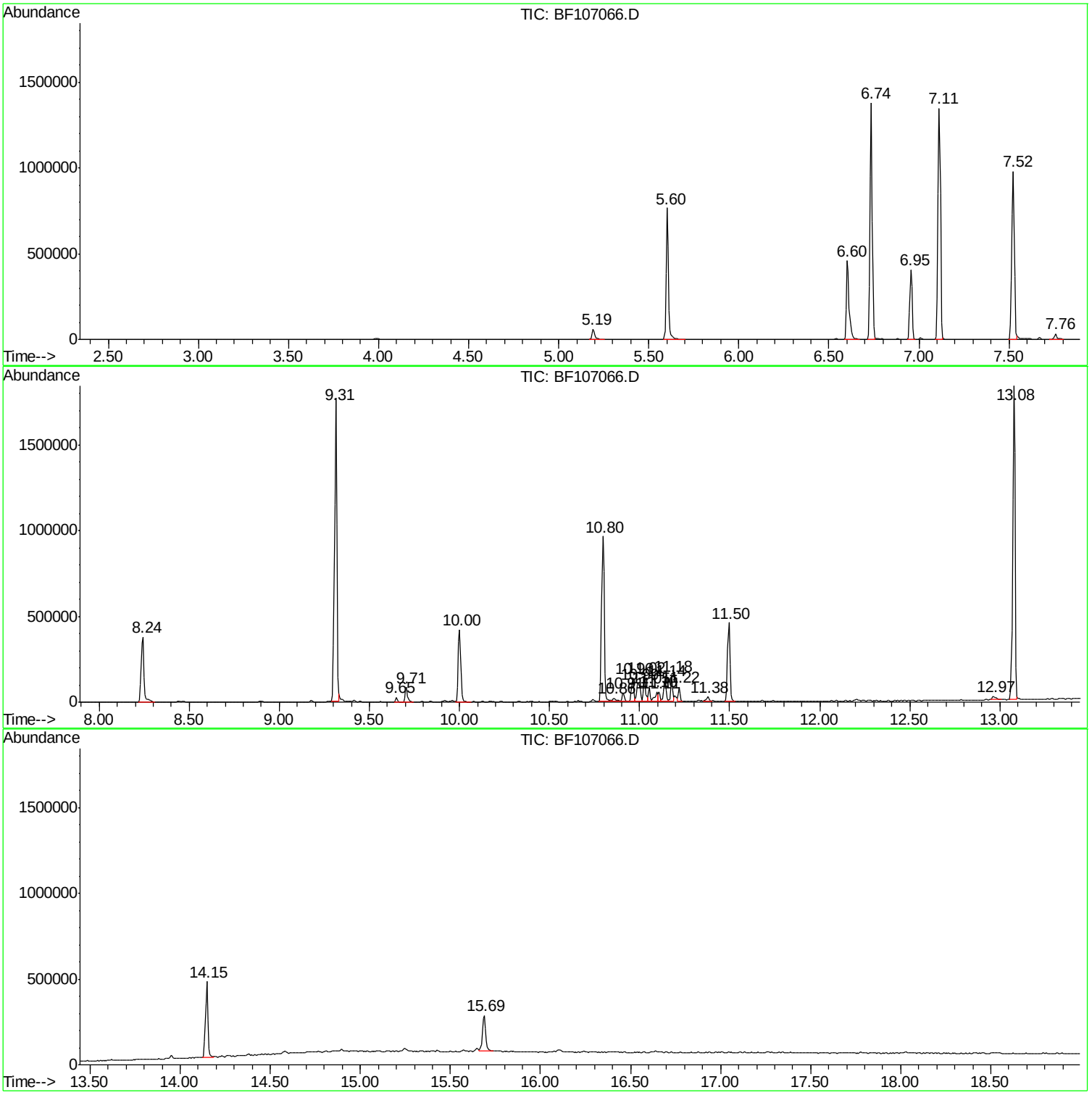
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070218\
Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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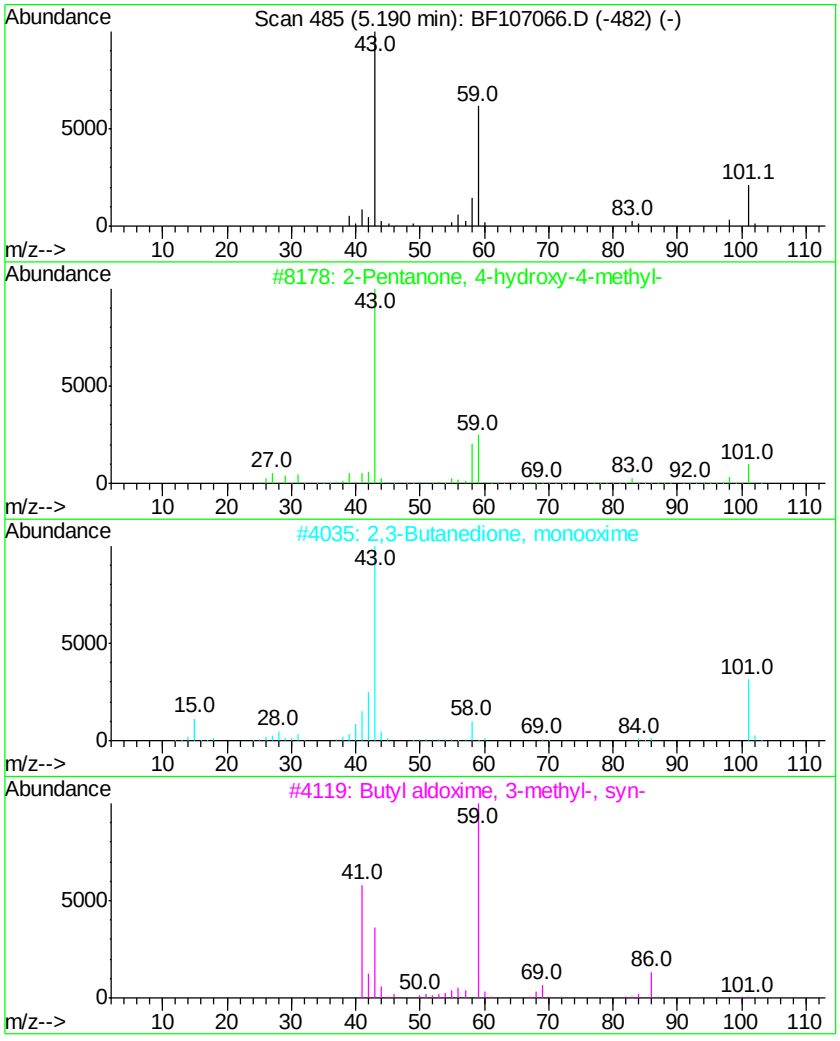
TIC Integration Parameters: LSCINT.P

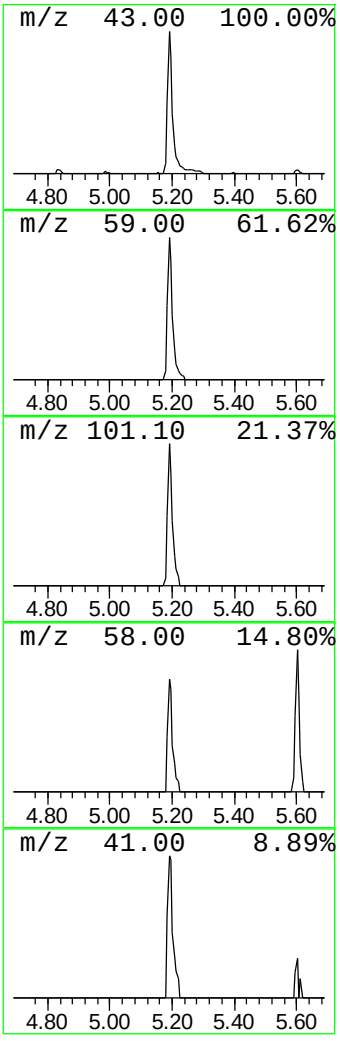
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	4.23 ng	71670	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

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Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

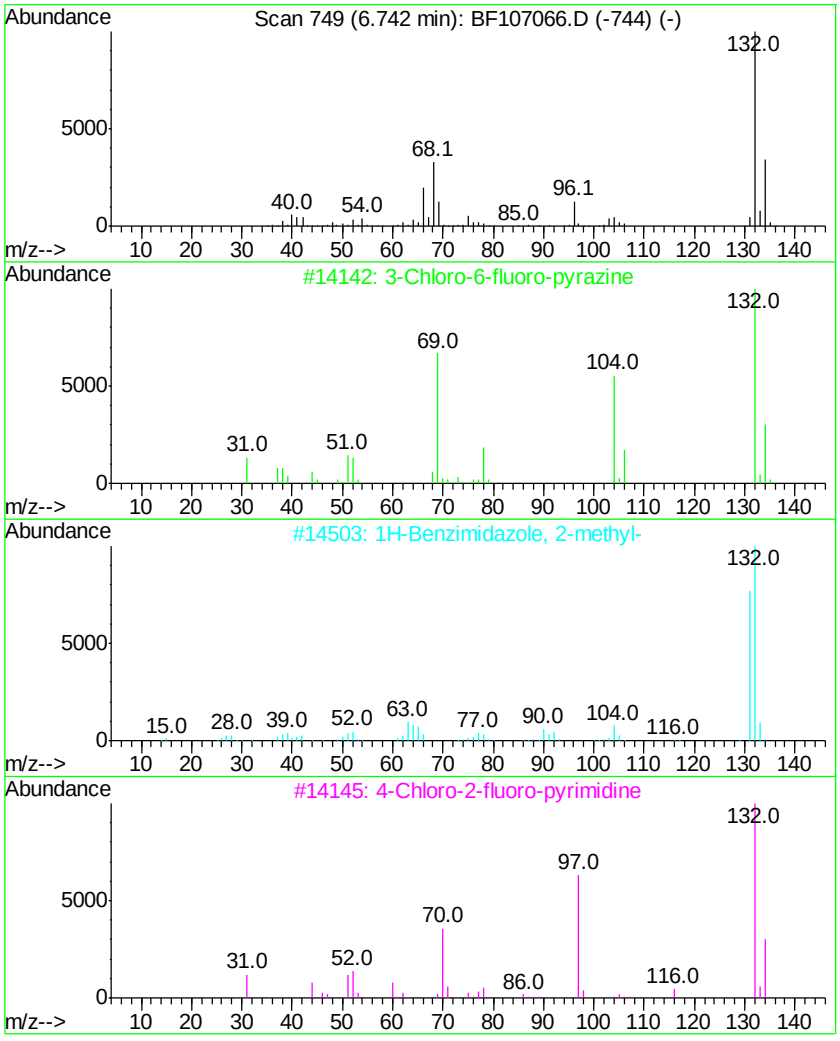
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

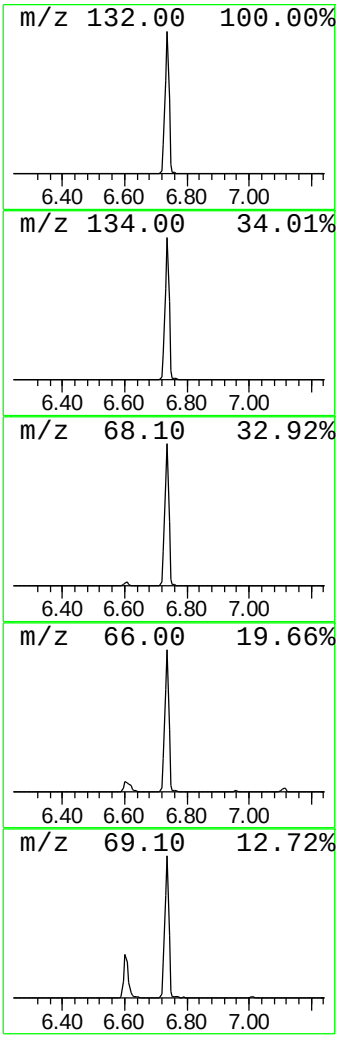
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	71.81 ng	1215850	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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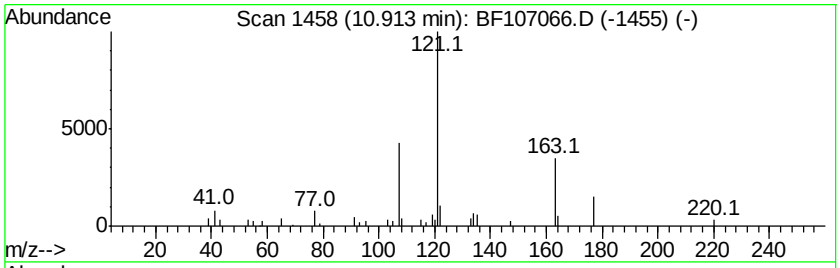
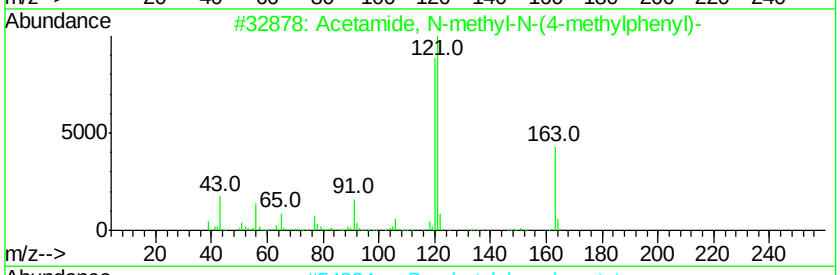
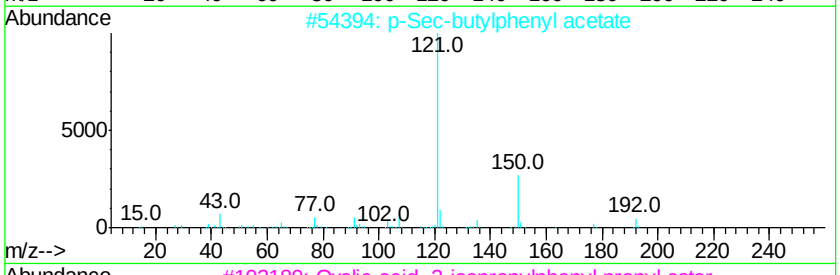
Peak Number 4 unknown10.91 Concentration Rank 12

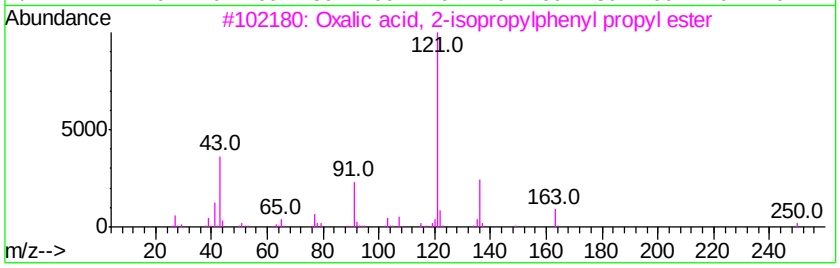
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.28 ng	44596	Phenanthrene-d10	11.50

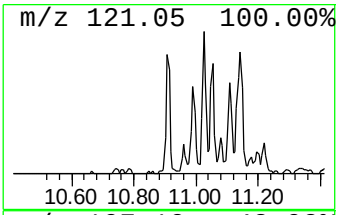
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-N-(4-methylp...	163	C10H13NO	000612-03-3	47
2	p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	43
3	Oxalic acid, 2-isopropylphenyl p...	250	C14H18O4	1000309-56-1	43
4	2H-1,2,3,4-Tetrazol-5-amine, N-[...	205	C9H11N5O	1000337-56-1	43
5	Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	38

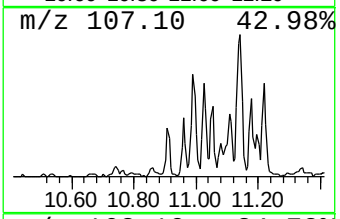


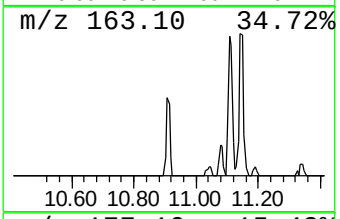


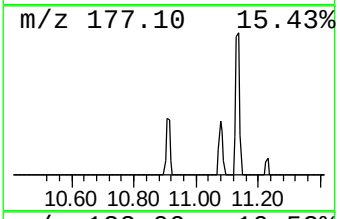


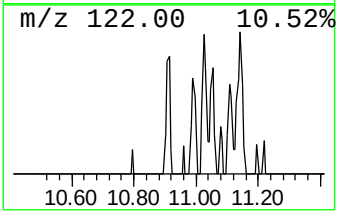












Library Search Compound Report

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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

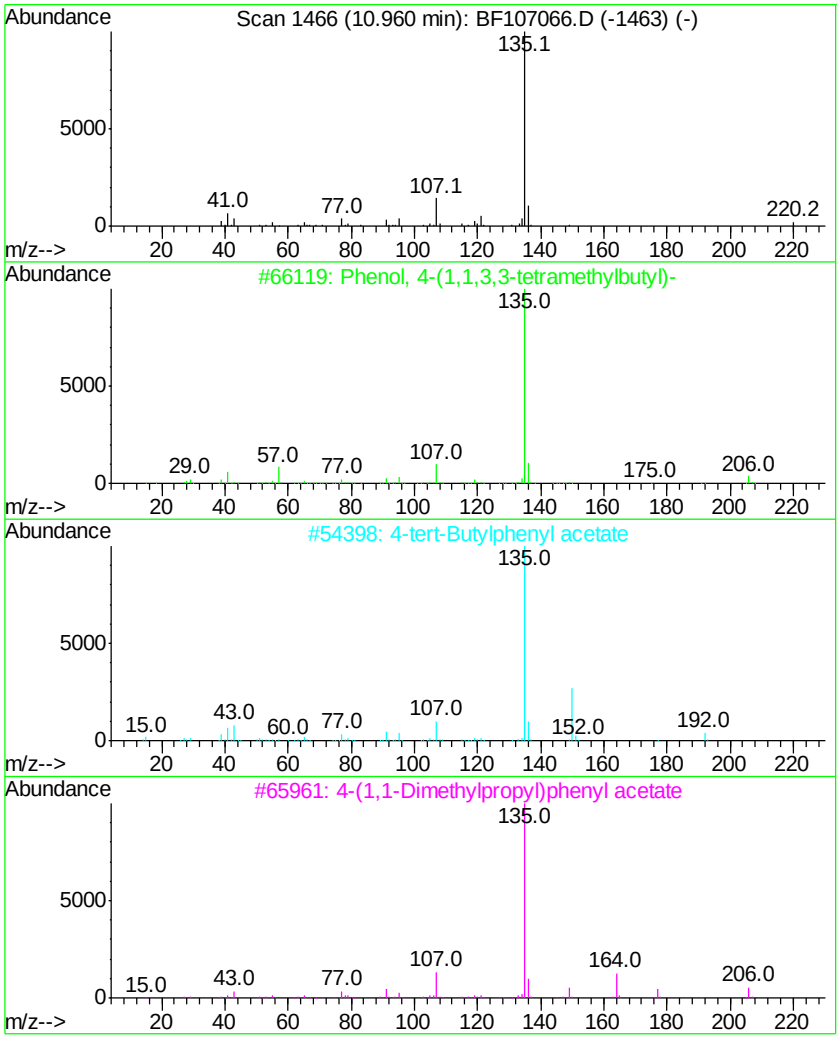
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

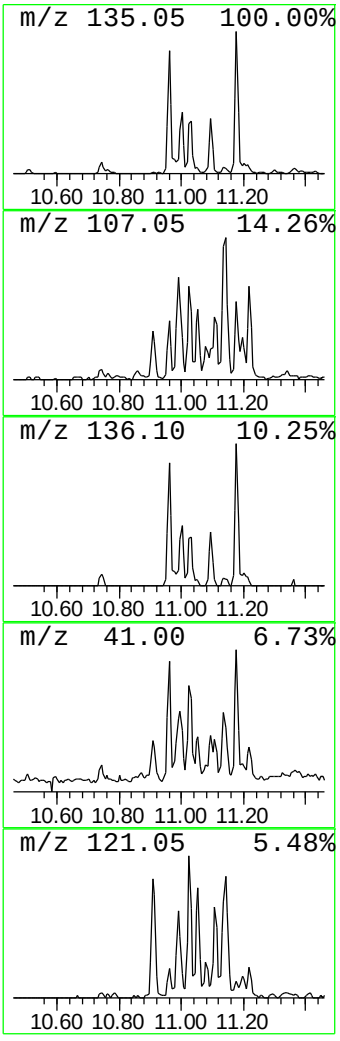
****

Peak Number 5 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	5.10 ng	99570	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	64
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	64
4	Benzoic acid, 4-methoxy-, diethy...	220	C12H17BO3	146681-61-0	59
5	Hexestrol	270	C18H22O2	000084-16-2	53





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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

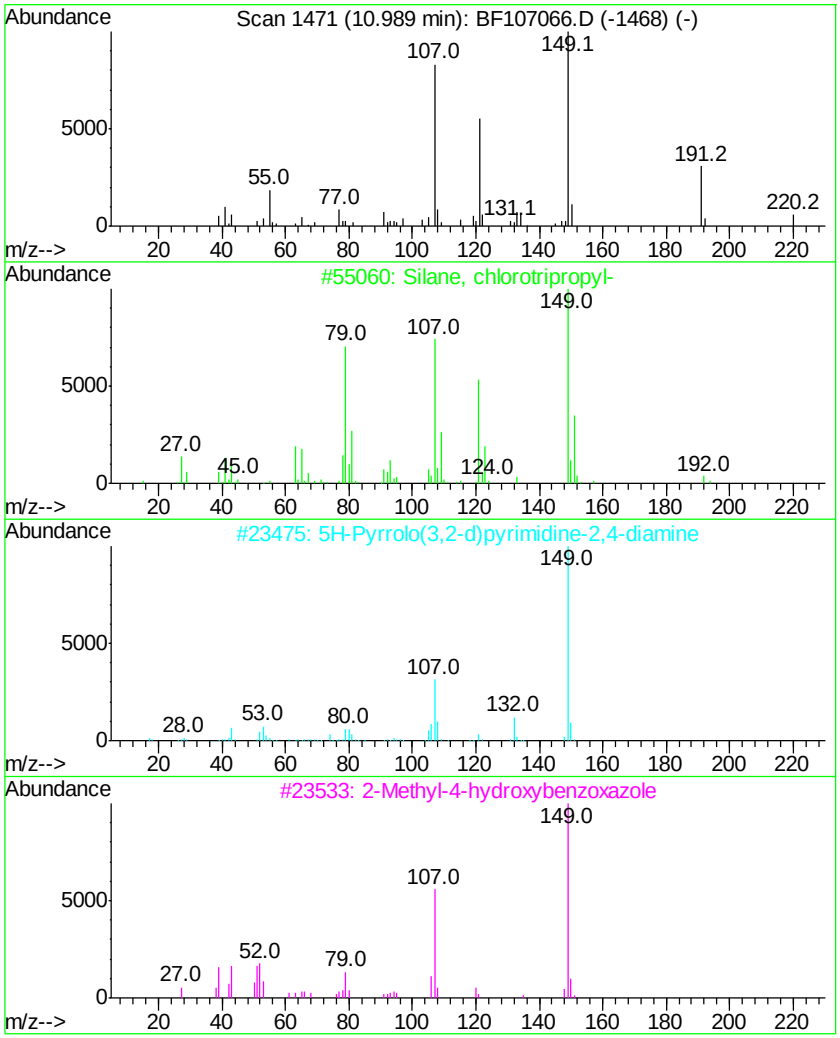
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

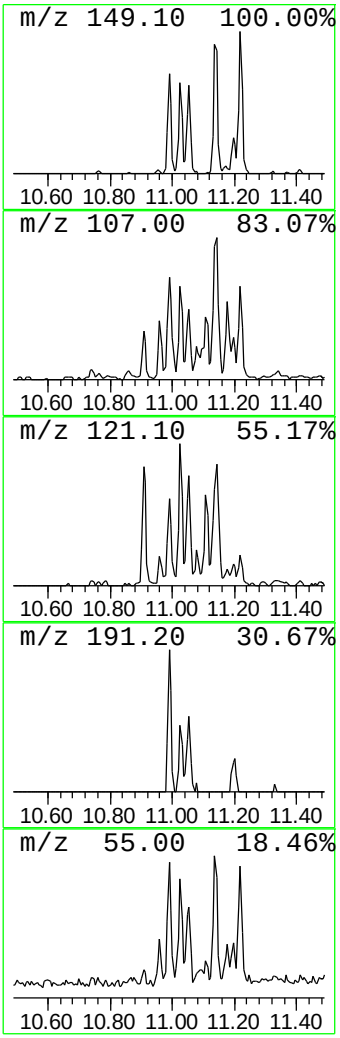
****

Peak Number 6 Silane, chlorotripropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	7.07 ng	137895	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	80
2	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	64
3	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	64
4	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	46
5	Butanamide, N-(4-methylphenyl)-3...	191	C11H13NO2	002415-85-2	38





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ALS Vial : 34 Sample Multiplier: 1

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TIC Library : C:\DATABASE\NIST11.L
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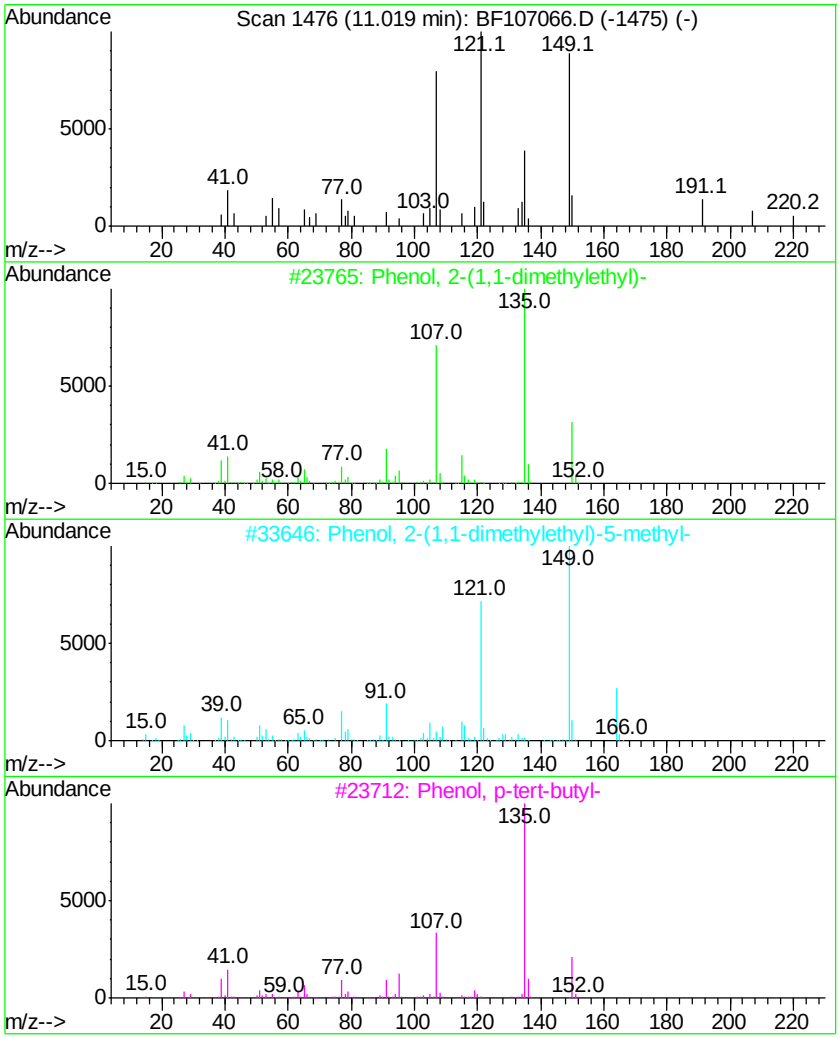
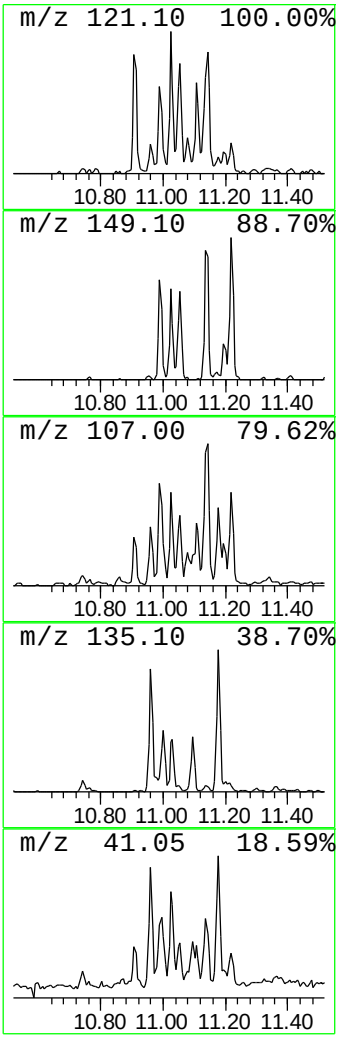
****

Peak Number 7 unknown11.02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	6.59 ng	128575	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	43
2	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	35
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	27
4	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	27
5	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	25





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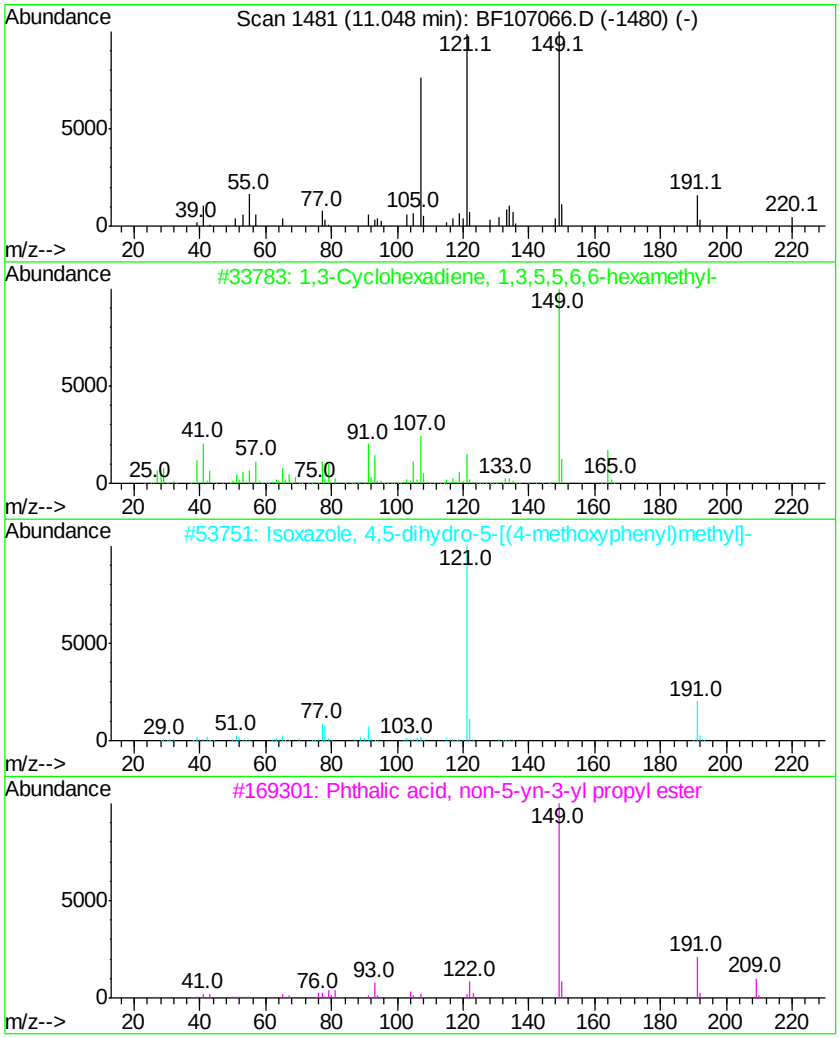
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

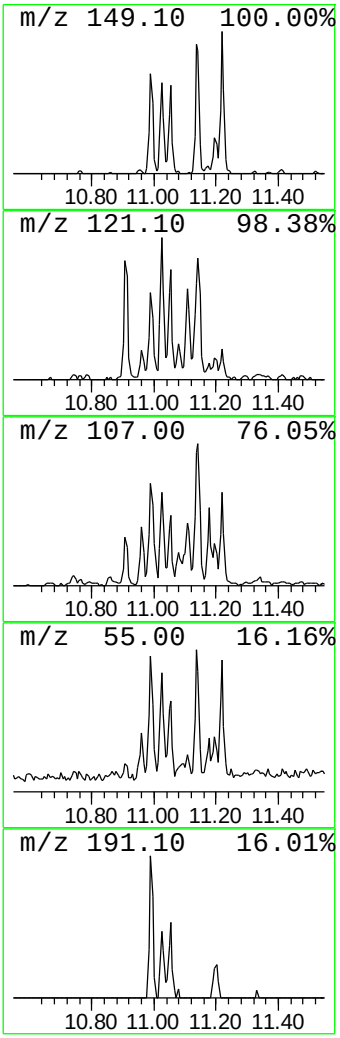
****

Peak Number 8 unknown11.05 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	3.09 ng	60303	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	43
2	Isoxazole, 4,5-dihydro-5-[(4-met...	191	C11H13NO2	1000362-14-0	30
3	Phthalic acid, non-5-yn-3-yl pro...	330	C20H26O4	1000315-18-1	25
4	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	25
5	Pyridine, 2,4,6-trimethyl-	121	C8H11N	000108-75-8	22





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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

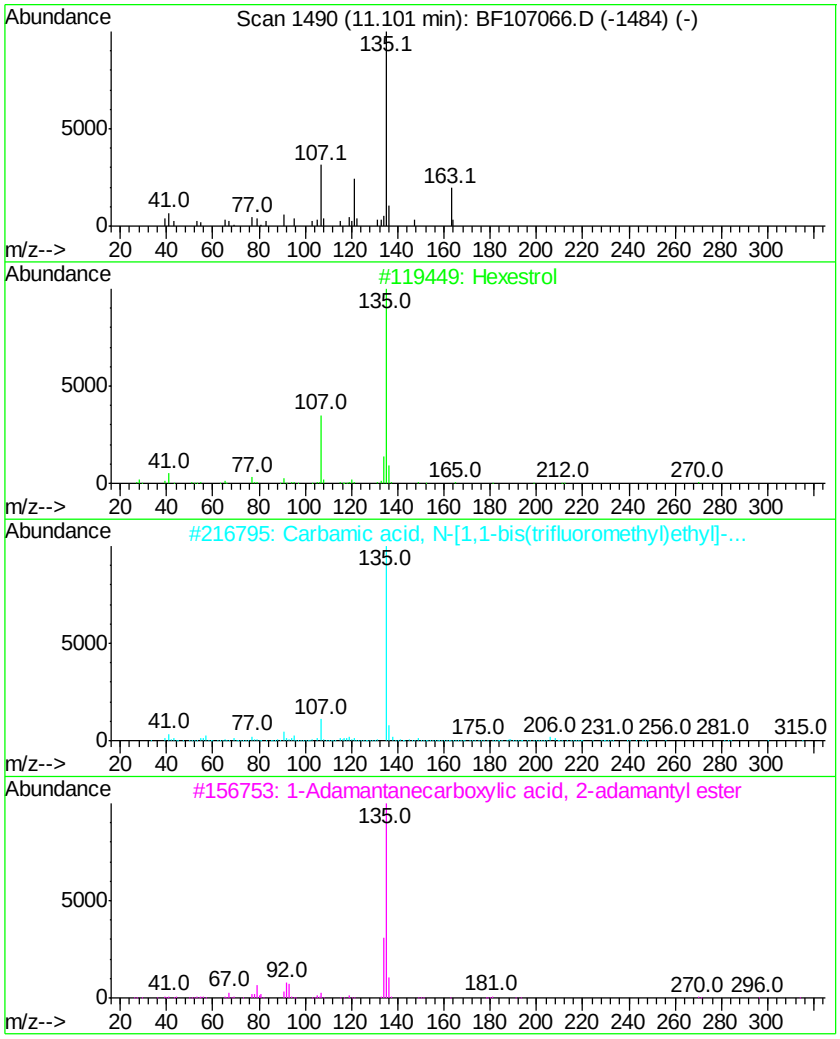
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

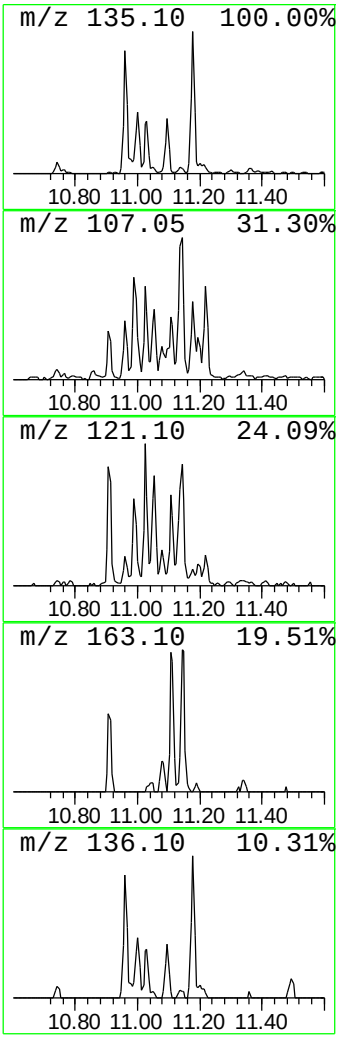
****

Peak Number 9 Hexestrol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	3.40 ng	66413	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexestrol	270	C18H22O2	000084-16-2	72
2	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	56
3	1-Adamantanecarboxylic acid, 2-a...	314	C21H30O2	1000282-94-3	50
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	45
5	3-Methoxybenzoic acid, 2,5-dichl...	296	C14H10Cl2O3	1000325-55-5	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070218\
Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

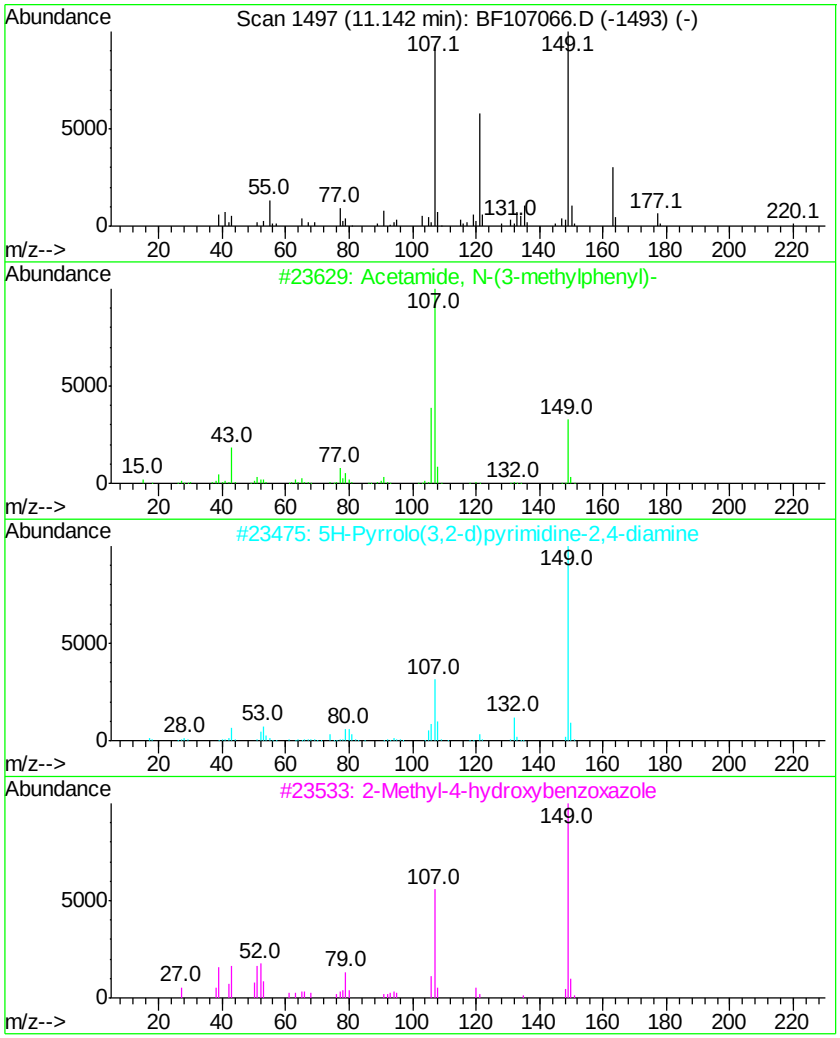
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

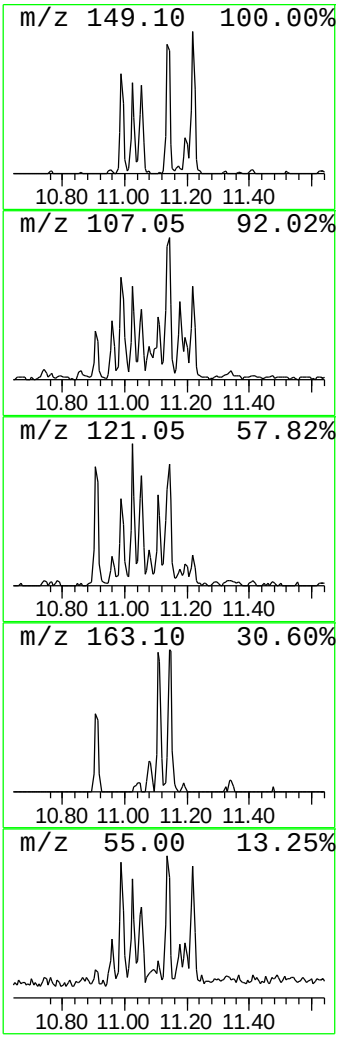
****

Peak Number 10 Acetamide, N-(3-methylphenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	7.09 ng	138299	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	64
2	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	64
3	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47
4	3-Methyl-4-(3,7,7-trimethyl-2-ox...	220	C14H20O2	1000189-10-9	38
5	p-Propionotoluidide	163	C10H13NO	002759-55-9	38





Library Search Compound Report

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Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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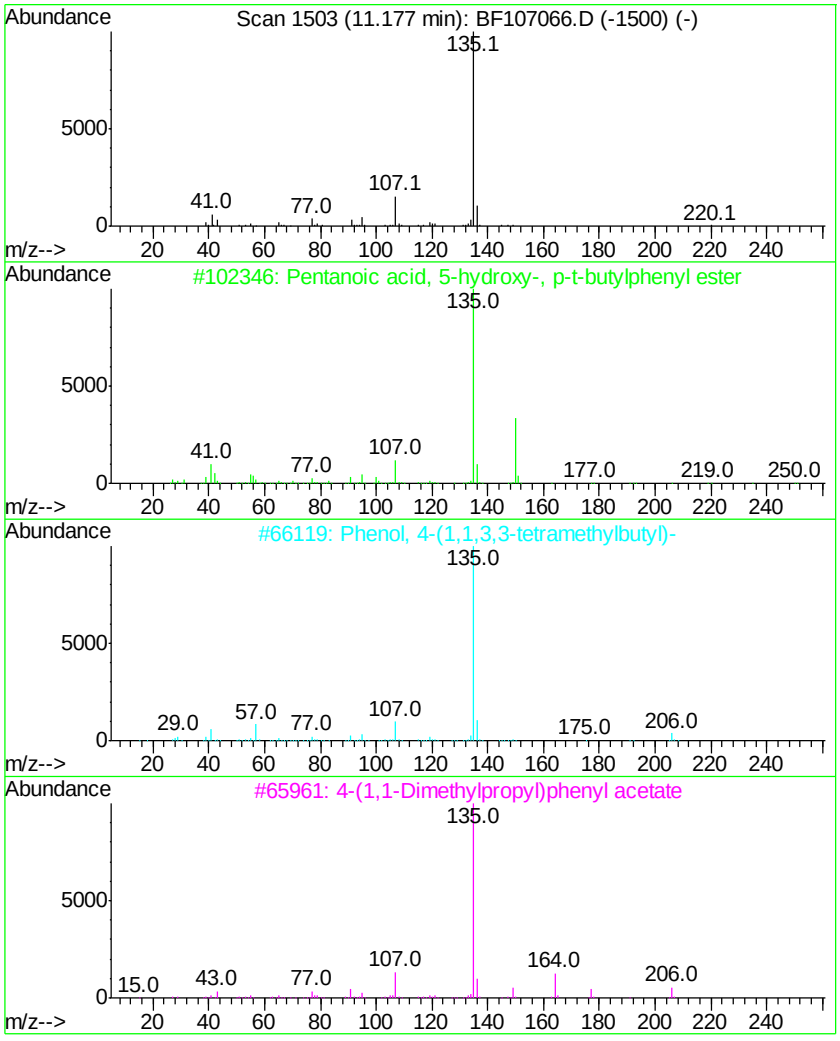
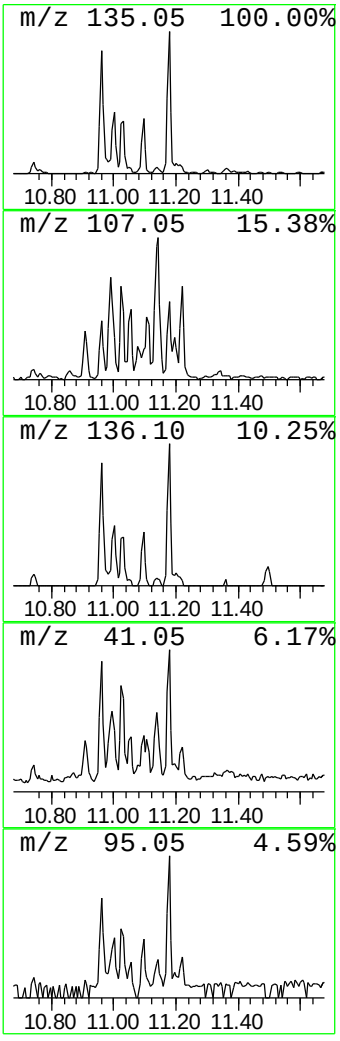
Peak Number 11 Pentanoic acid, 5-hydroxy-,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	6.09 ng	118804	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	78
2	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
4	Hexestrol	270	C18H22O2	000084-16-2	72
5	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	64





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Data File : BF107066.D
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Operator : JU/SJ
Sample : J3800-08
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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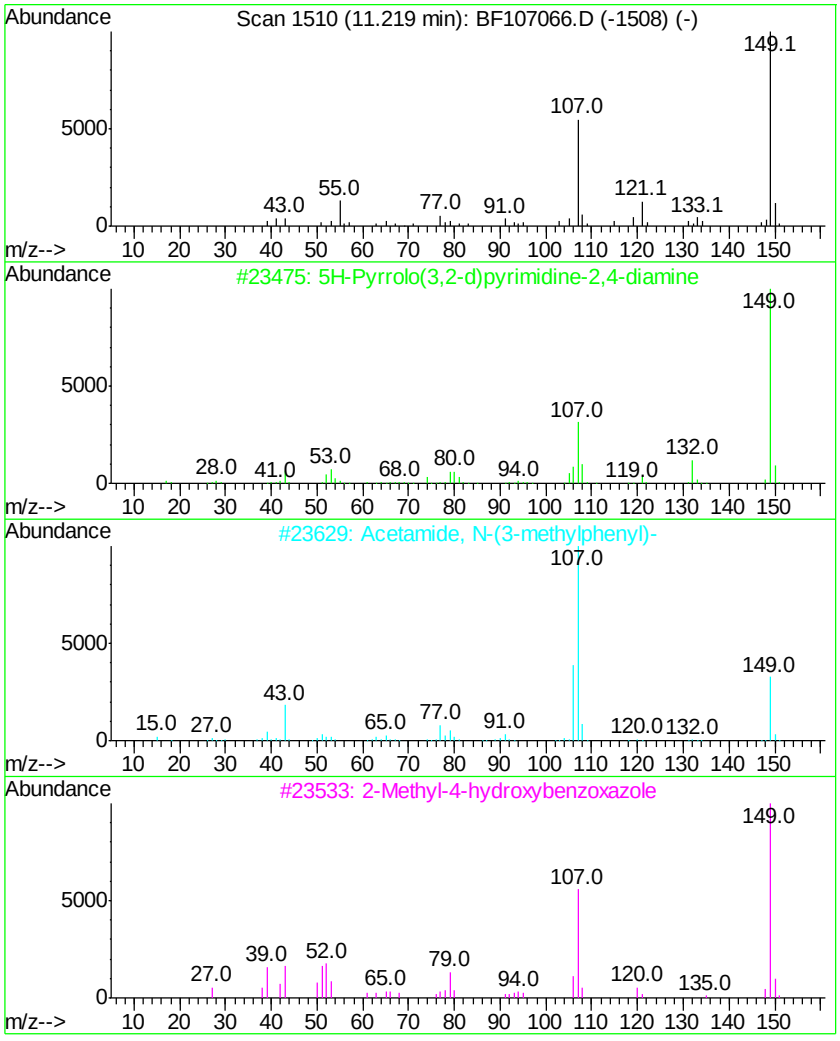
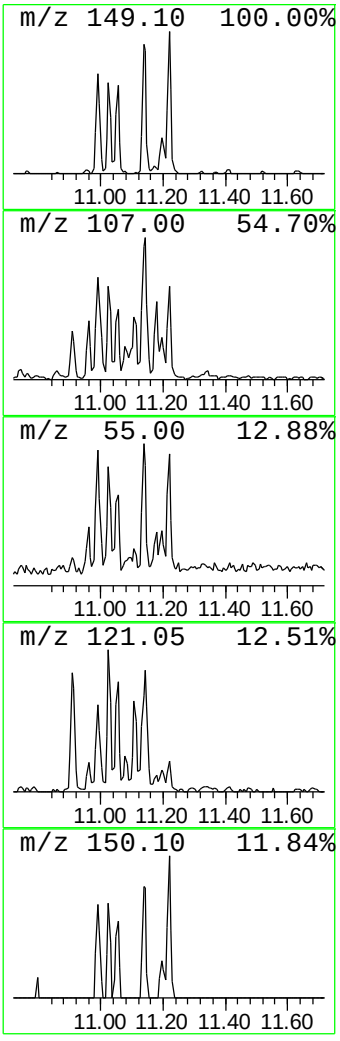
Peak Number 12 5H-Pyrrolo(3,2-d)pyrimidine... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	3.29 ng	64259	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	72
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	72
3	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	72
4	6-Amino-1-methylpurine	149	C6H7N5	005142-22-3	53
5	Phthalic acid, isobutyl tridec-2...	400	C25H36O4	1000315-44-3	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070218\
Data File : BF107066.D
Acq On : 3 Jul 2018 2:30
Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : MW-14

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	4.2	ng	71670	1	6.95	338610	20.0
unknown6.74	6.74	71.8	ng	1215850	1	6.95	338610	20.0
unknown10.91	10.91	2.3	ng	44596	4	11.50	390356	20.0
Phenol, 4-(1,1,3,...	10.96	5.1	ng	99570	4	11.50	390356	20.0
Silane, chlorotri...	10.99	7.1	ng	137895	4	11.50	390356	20.0
unknown11.02	11.02	6.6	ng	128575	4	11.50	390356	20.0
unknown11.05	11.05	3.1	ng	60303	4	11.50	390356	20.0
Hexestrol	11.10	3.4	ng	66413	4	11.50	390356	20.0
Acetamide, N-(3-m...	11.14	7.1	ng	138299	4	11.50	390356	20.0
Pentanoic acid, 5...	11.18	6.1	ng	118804	4	11.50	390356	20.0
5H-Pyrrolo(3,2-d)...	11.22	3.3	ng	64259	4	11.50	390356	20.0