LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.747	13	14	23	rVB	142234	281943	4.21%	1.267%
2	1.872	23	25	79	rVB	2847014	6698078	100.00%	30.096%
3	5.393	331	333	336	rBV	918333	839410	12.53%	3.772%
4	6.444	422	425	427	rBV	724802	917902	13.70%	4.124%
5	6.570	434	436	439	rBV	875132	934069	13.95%	4.197%
6	6.810	455	457	459	rBV	948348	765344	11.43%	3.439%
7	6.970	468	471	473	rVB	717486	793330	11.84%	3.565%
8	7.370	504	506	508	rBV	693253	588186	8.78%	2.643%
9	8.102	567	570	572	rBV	1080817	1040647	15.54%	4.676%
10	9.176	661	664	666	rBV	1179215	1149738	17.17%	5.166%
11	9.565	696	698	700	rVB	110134	88134	1.32%	0.396%
12	9.850	720	723	724	rBV	1168762	1066996	15.93%	4.794%
13	10.628	789	791	794	rBV	639352	547855	8.18%	2.462%
14	11.325	850	852	853	rBV	977608	808047	12.06%	3.631%
15	11.348	853	854	856	rVV	241880	185956	2.78%	0.836%
16	12.525	955	957	959	rBV	200304	218739	3.27%	0.983%
17	12.754	973	977	980	rBV	218181	275259	4.11%	1.237%
18	12.902	988	990	993	rVB	751623	667288	9.96%	2.998%
19	13.954	1079	1082	1083	rBV2	794587	992201	14.81%	4.458%
20	14.434	1122	1124	1127	rVV3	84994	120083	1.79%	0.540%
21	14.708	1146	1148	1153	rBV4	36885	71936	1.07%	0.323%
22	14.959	1168	1170	1174	rVV	123866	240833	3.60%	1.082%
23	15.051	1175	1178	1182	rVV2	176383	273173	4.08%	1.227%
24	15.234	1192	1194	1197	rVB	65340	98518	1.47%	0.443%
25	15.302	1197	1200	1202	rBV	79345	137482	2.05%	0.618%
26	15.359	1202	1205	1207	rBV	544639	662125	9.89%	2.975%
27	15.805	1242	1244	1247	rBV	169533	294244	4.39%	1.322%
28	16.708	1321	1323	1325	rBV	41584	75418	1.13%	0.339%
29	16.765	1326	1328	1331	rVB	52788	100372	1.50%	0.451%
30	17.120	1357	1359	1365	rVB	37616	80723	1.21%	0.363%
31	17.268	1369	1372	1384	rVB8	105325	399665	5.97%	1.796%
32	17.703	1407	1410	1415	rBV2	34184	135883	2.03%	0.611%
33	17.794	1415	1418	1422	rVB4	50623	138469	2.07%	0.622%
34	18.023	1434	1438	1446	rBV8	50249	251748	3.76%	1.131%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.188	1535	1540	1547	rVB2	93482	315598	4.71%	1.418%

Sum of corrected areas: 22255392

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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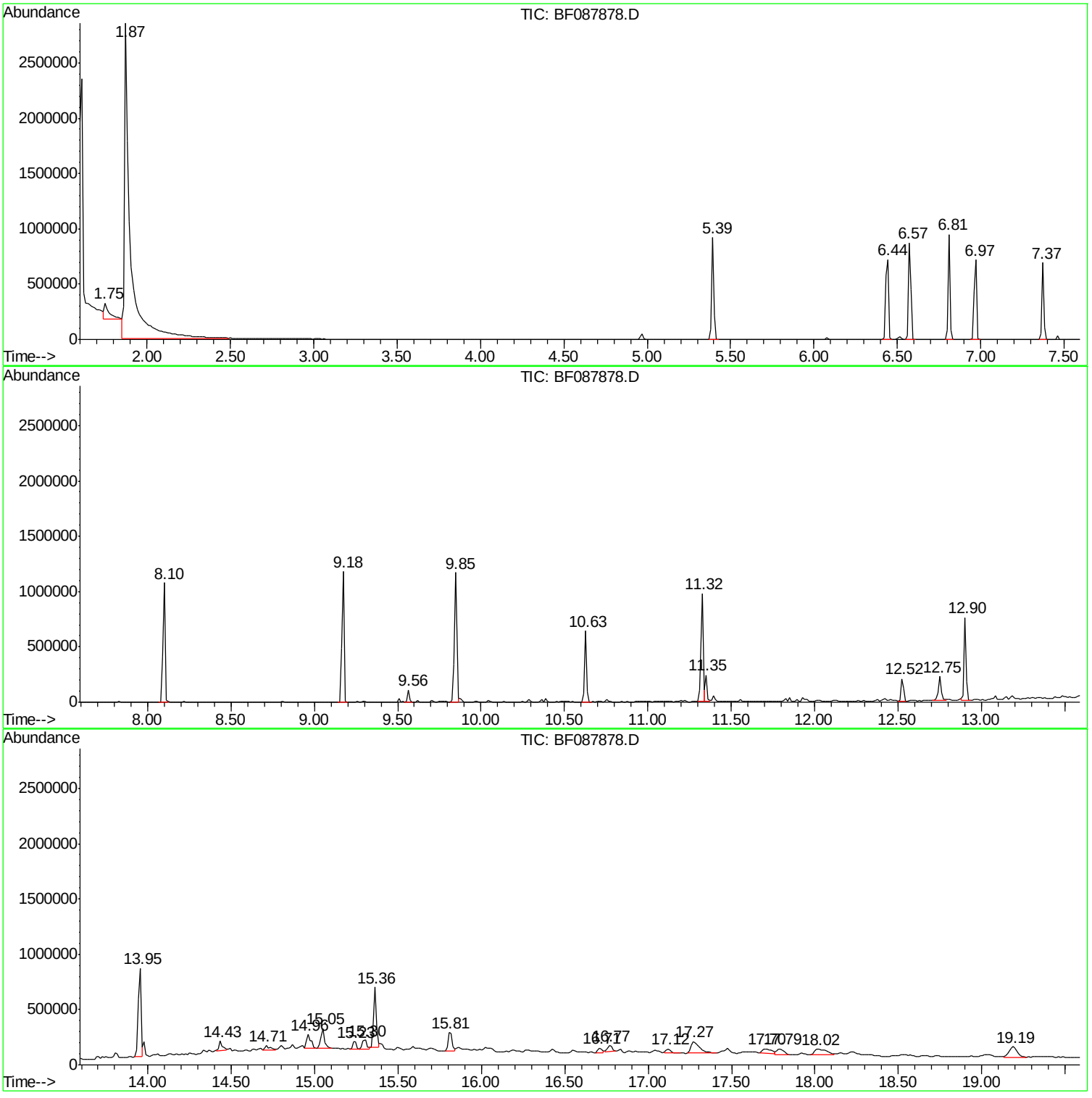
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

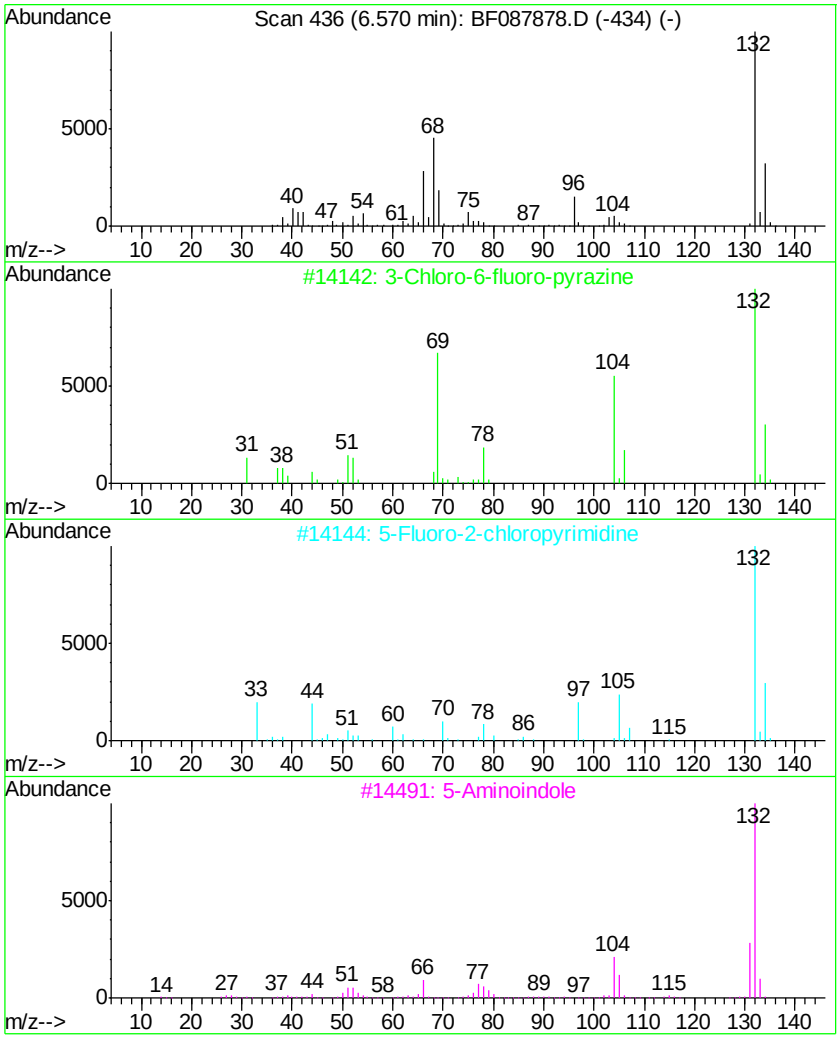
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

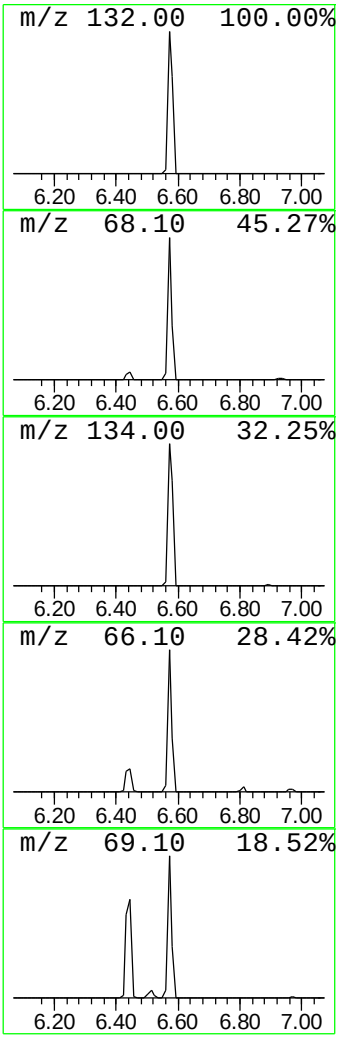
****

Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	23.55 ng	934069	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

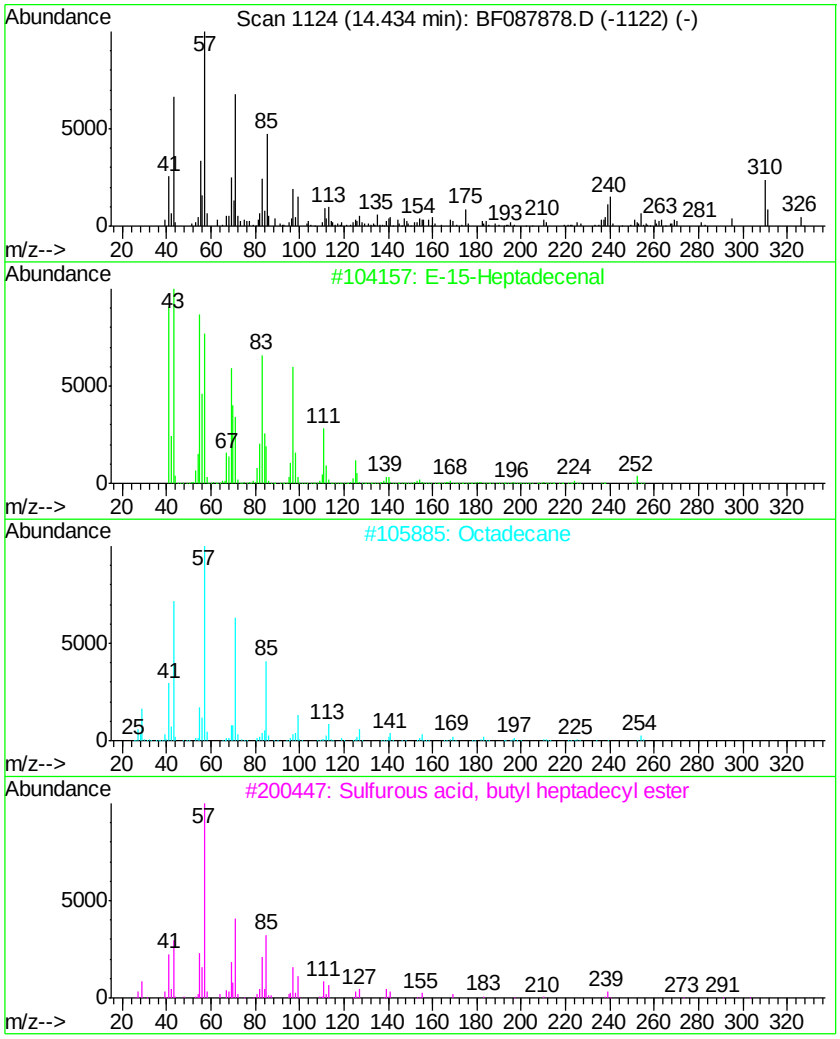
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

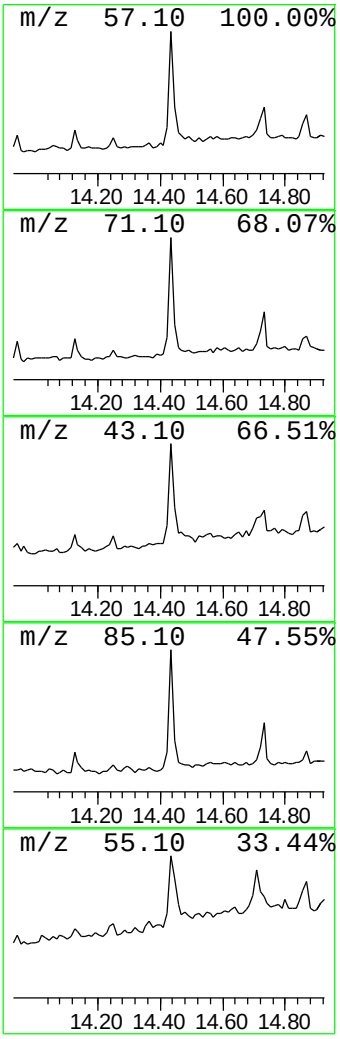
****

Peak Number 5 E-15-Heptadecenal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.42 ng	120083	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
2	Octadecane	254	C18H38	000593-45-3	70
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
4	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	64
5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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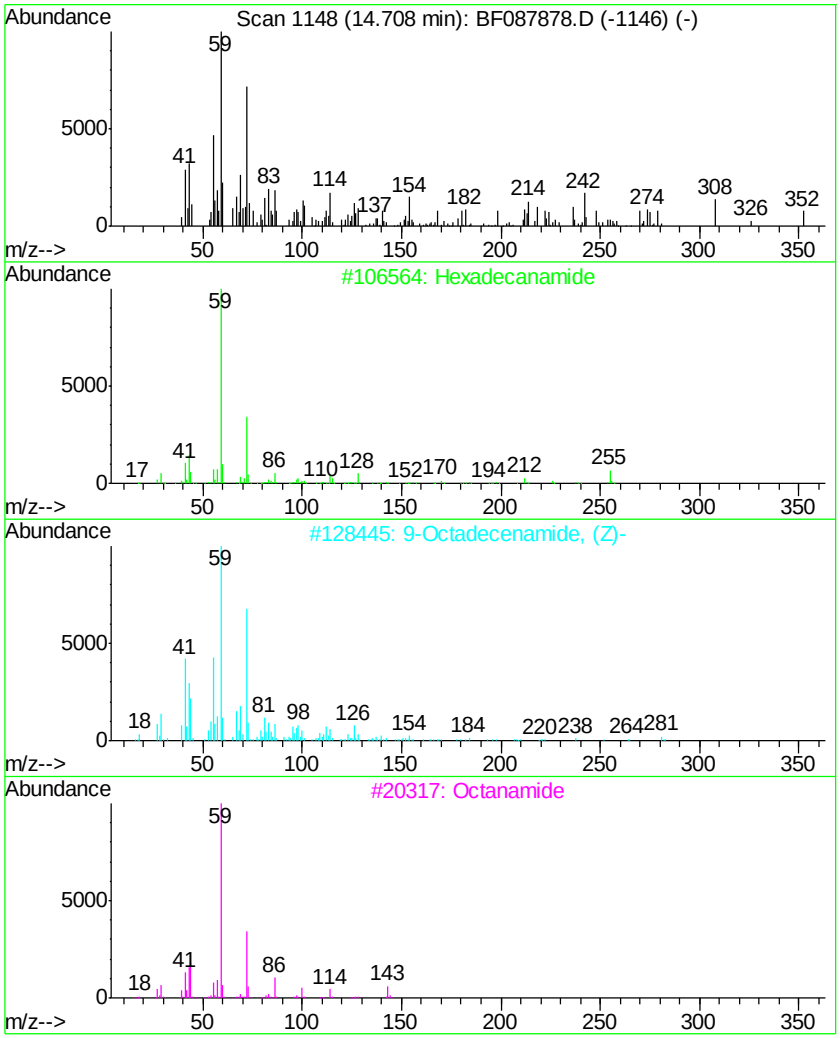
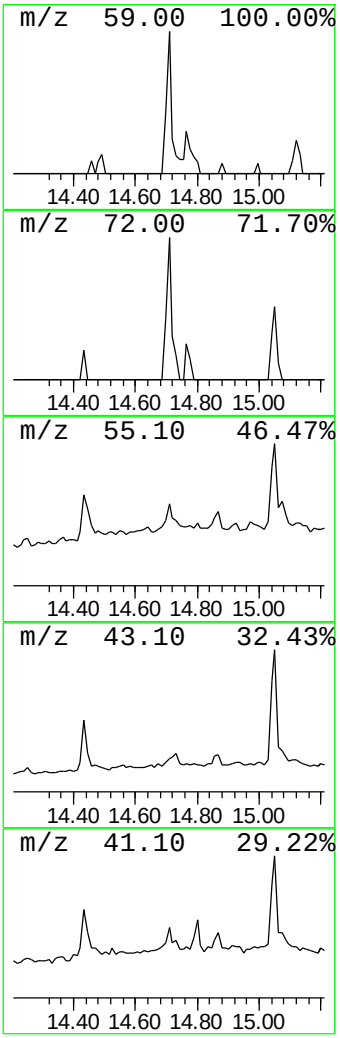
Peak Number 6 Hexadecanamide Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.17 ng	71936	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	58
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
3	Octanamide	143	C8H17NO	000629-01-6	53
4	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	50
5	Dodecanamide	199	C12H25NO	001120-16-7	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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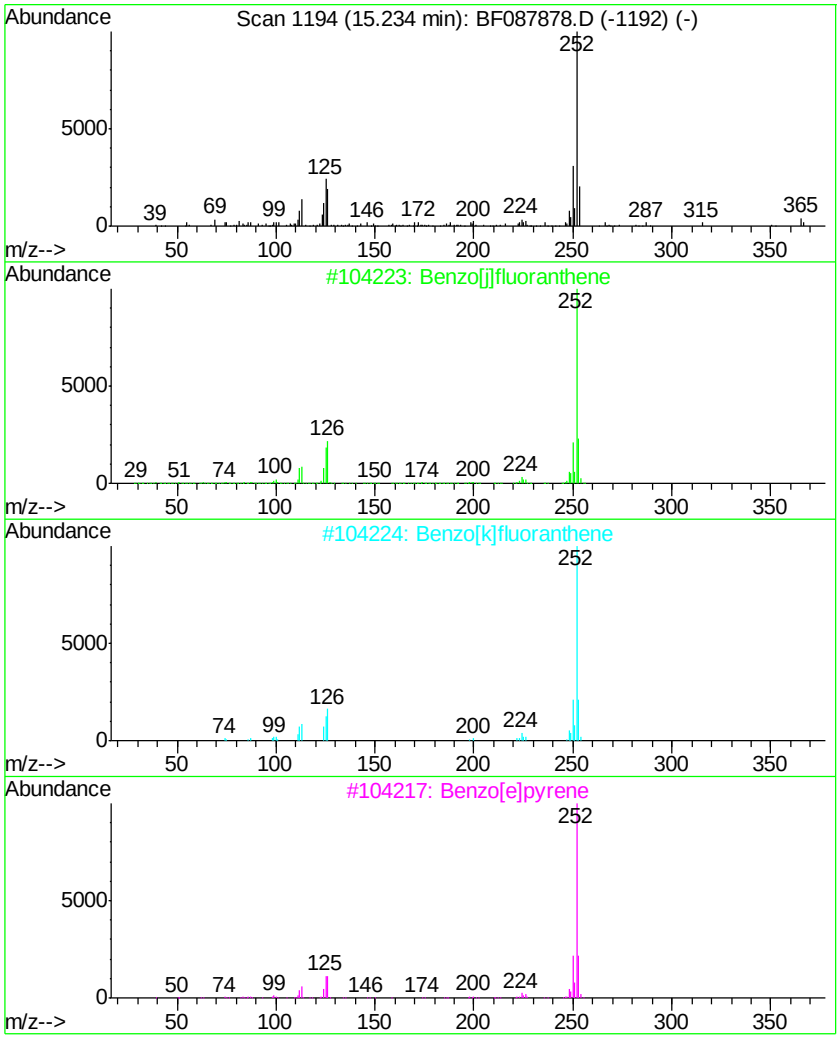
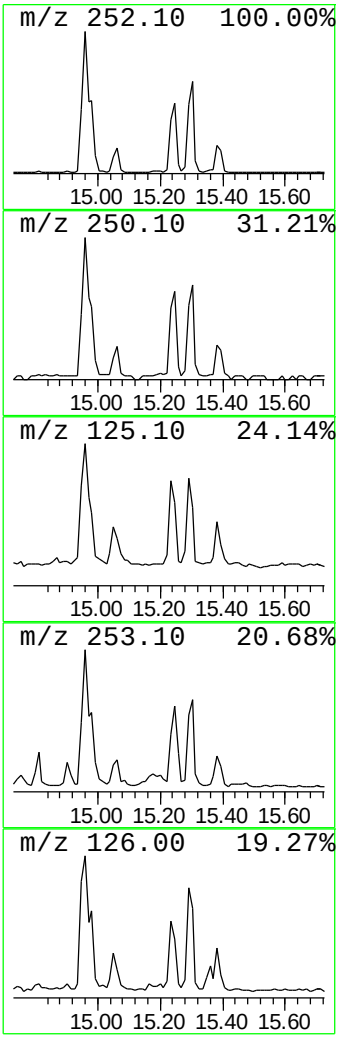
Peak Number 8 Benzo[j]fluoranthene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	2.98 ng	98518	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[e]pyrene	252	C20H12	000192-97-2	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	96





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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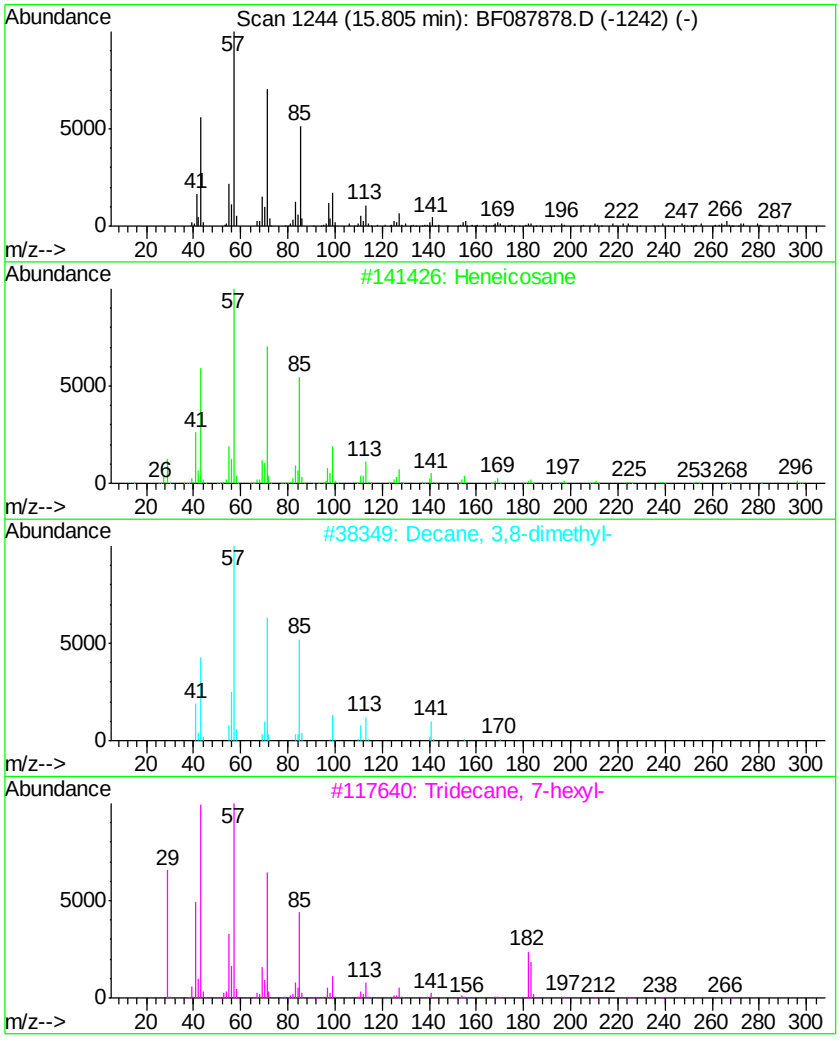
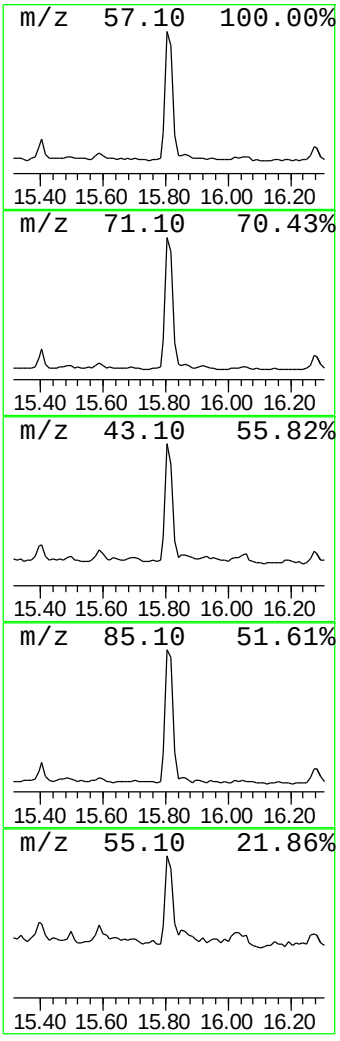
Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	8.89 ng	294244	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	87
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Octadecane	254	C18H38	000593-45-3	83





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Acq On : 10 Jun 2016 16:56
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Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

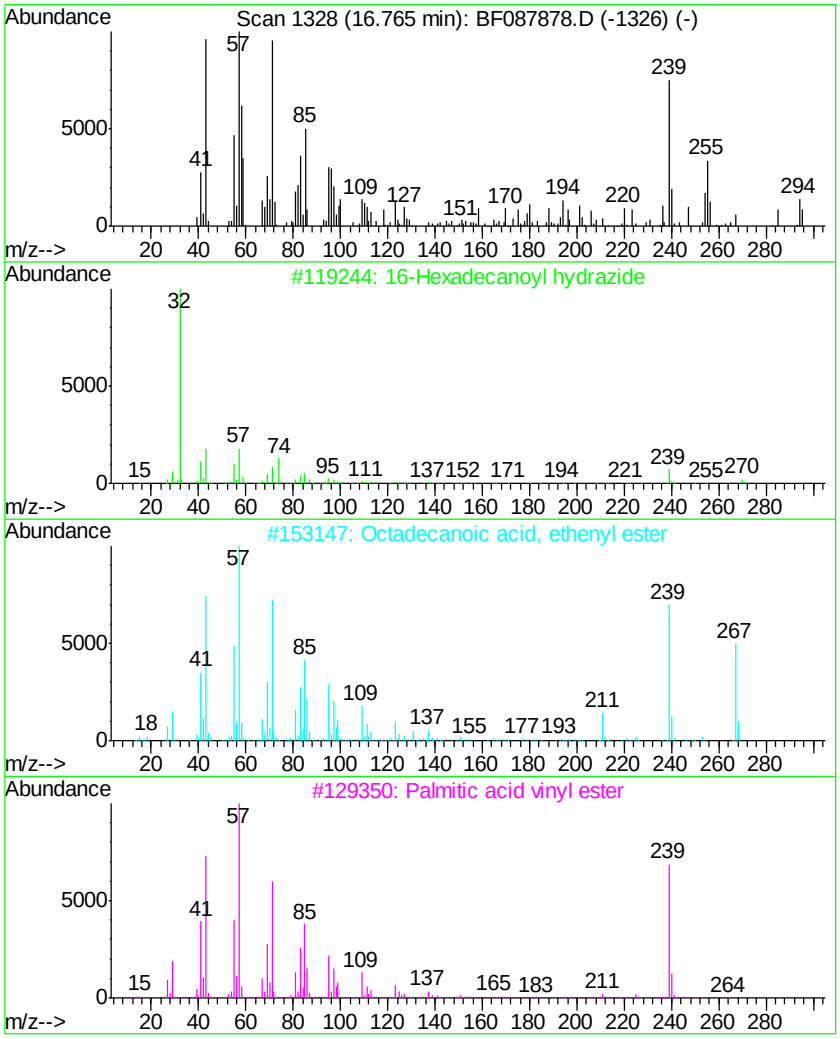
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

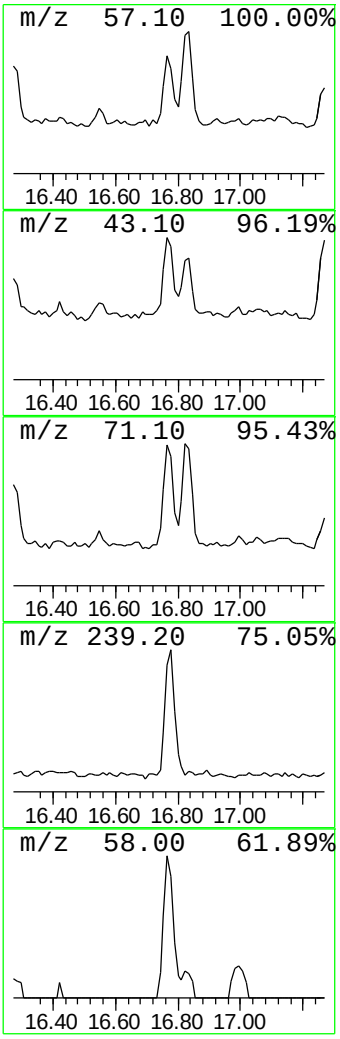
****

Peak Number 11 16-Hexadecanoyl hydrazide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.77	3.03 ng	100372	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	58
2	Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	58
3	Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	46
4	Decane, 3-methyl-	156	C11H24	013151-34-3	30
5	Tetradecane	198	C14H30	000629-59-4	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

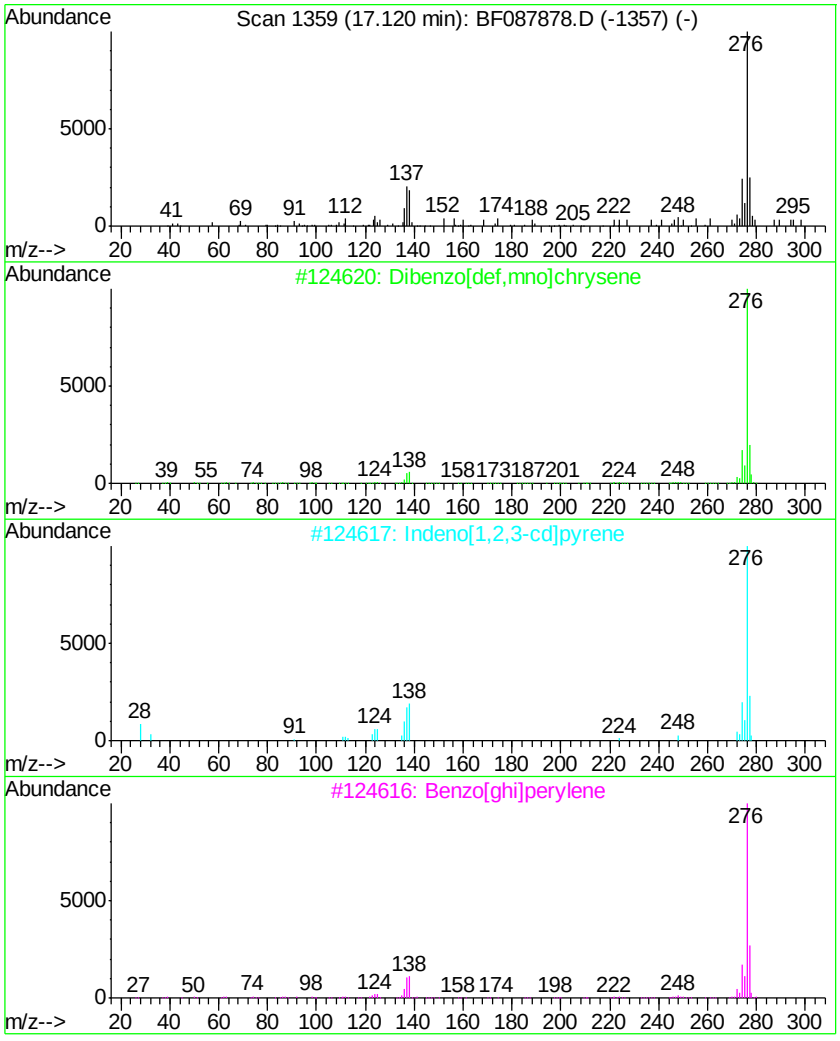
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

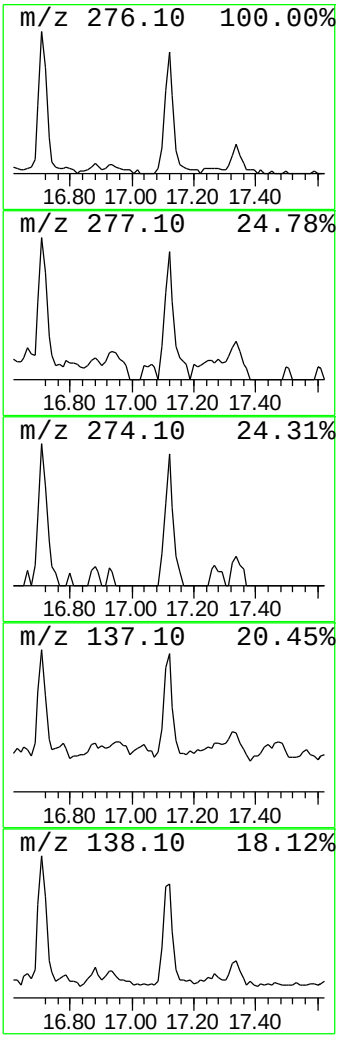
****

Peak Number 12 Dibenzo[def,mno]chrysene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.12	2.44 ng	80723	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	94
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	93
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	90
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	62
5	Benzofuro[3,2-d]pyrimidine, 4-me...	276	C17H12N2O2	312265-36-4	50





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ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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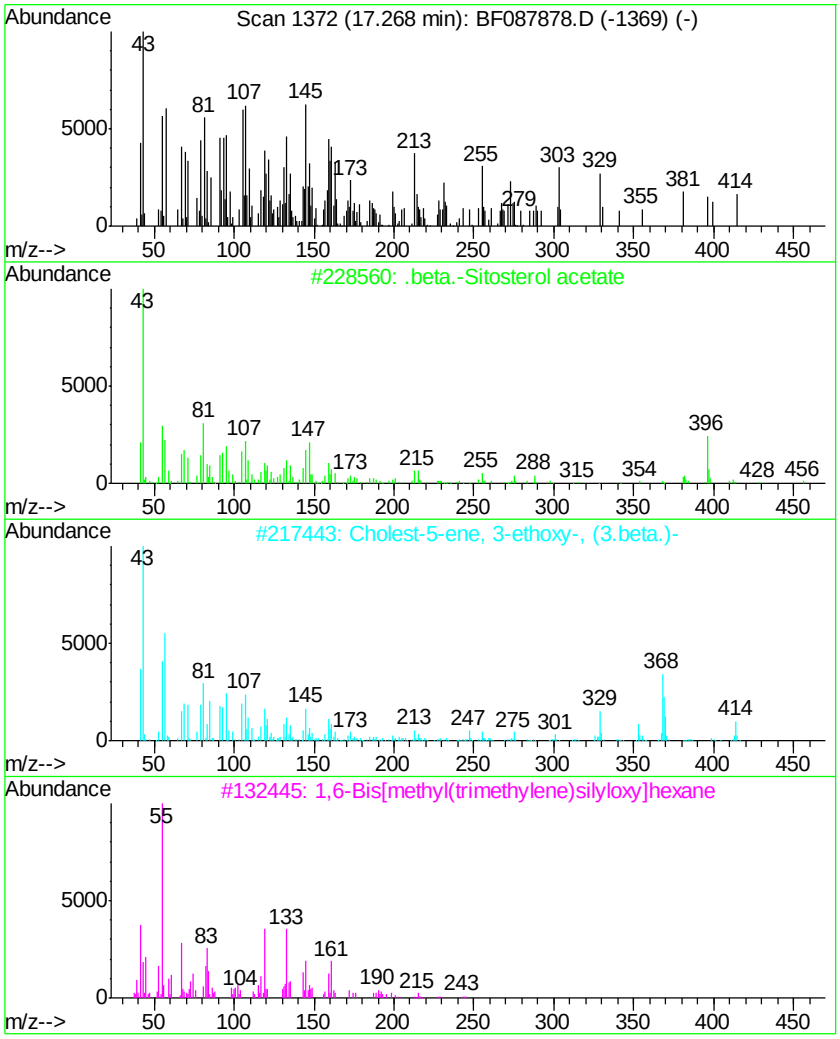
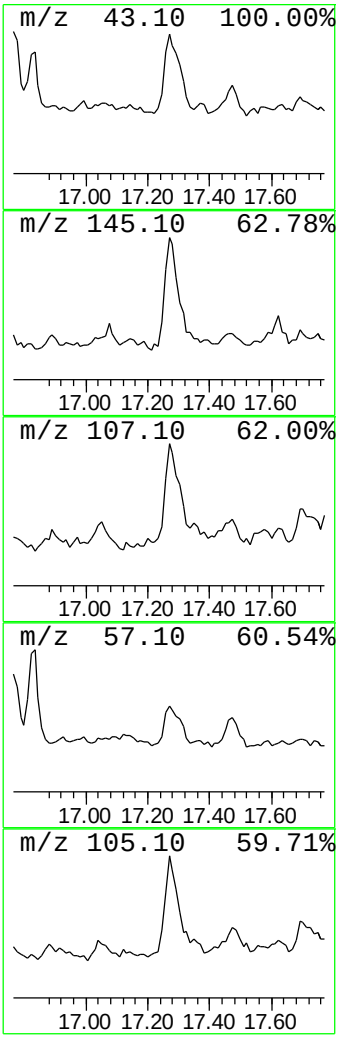
Peak Number 13 .beta.-Sitosterol acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.27	12.07 ng	399665	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	52
2	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	43
3	1,6-Bis[methyl(trimethylene)silv...	286	C14H30O2Si2	1000217-00-5	32
4	Bicyclo[2.2.1]heptane, 2-cyclopr...	176	C13H20	1000159-45-7	30
5	Stigmastan-3,5-diene	396	C29H48	1000214-16-4	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

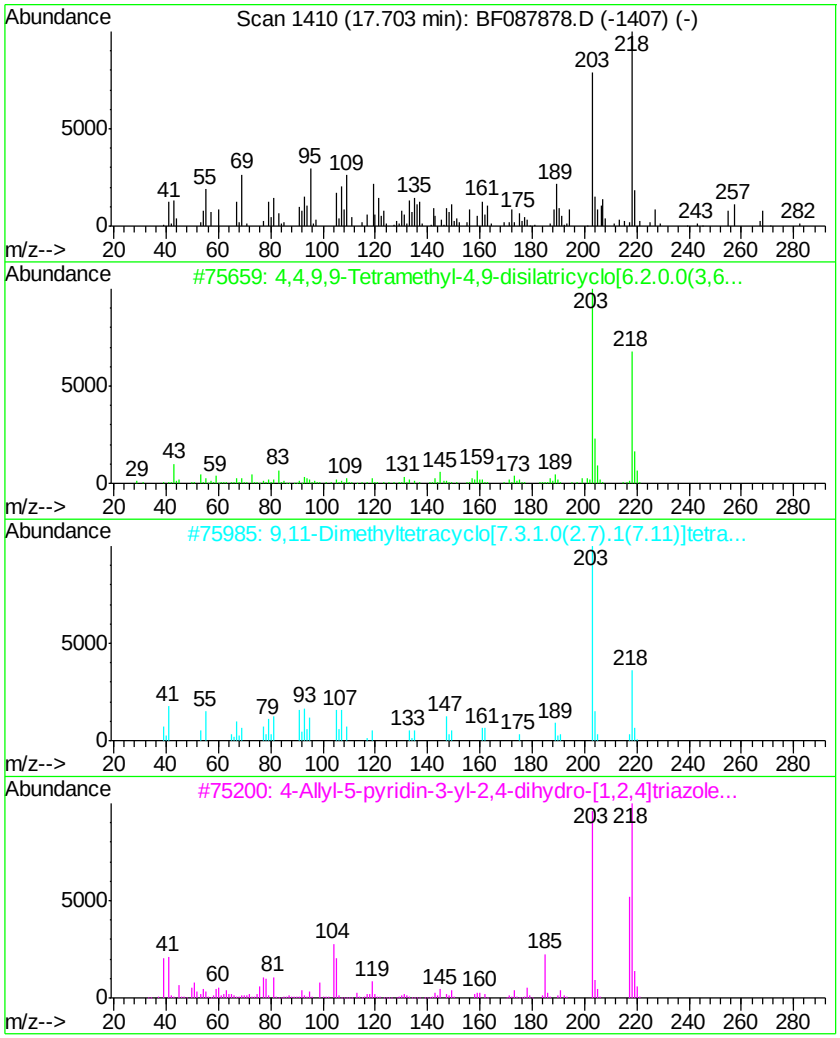
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

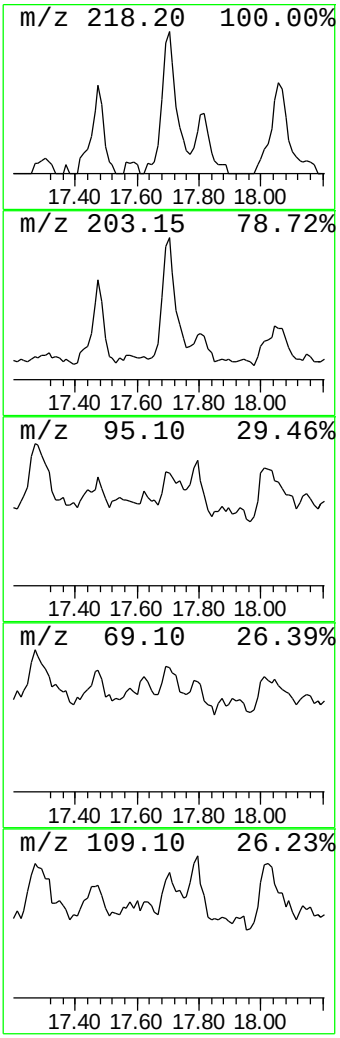
****

Peak Number 14 unknown17.70 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	4.10 ng	135883	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4,9,9-Tetramethyl-4,9-disilatr...	218	C12H18Si2	1000280-67-7	43
2	9,11-Dimethyltetracyclo[7.3.1.0(...	218	C16H26	053263-99-3	43
3	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	43
4	2H-1-Benzopyran-2-one, 7-acetyl-...	260	C14H12O5	129812-32-4	43
5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	38





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Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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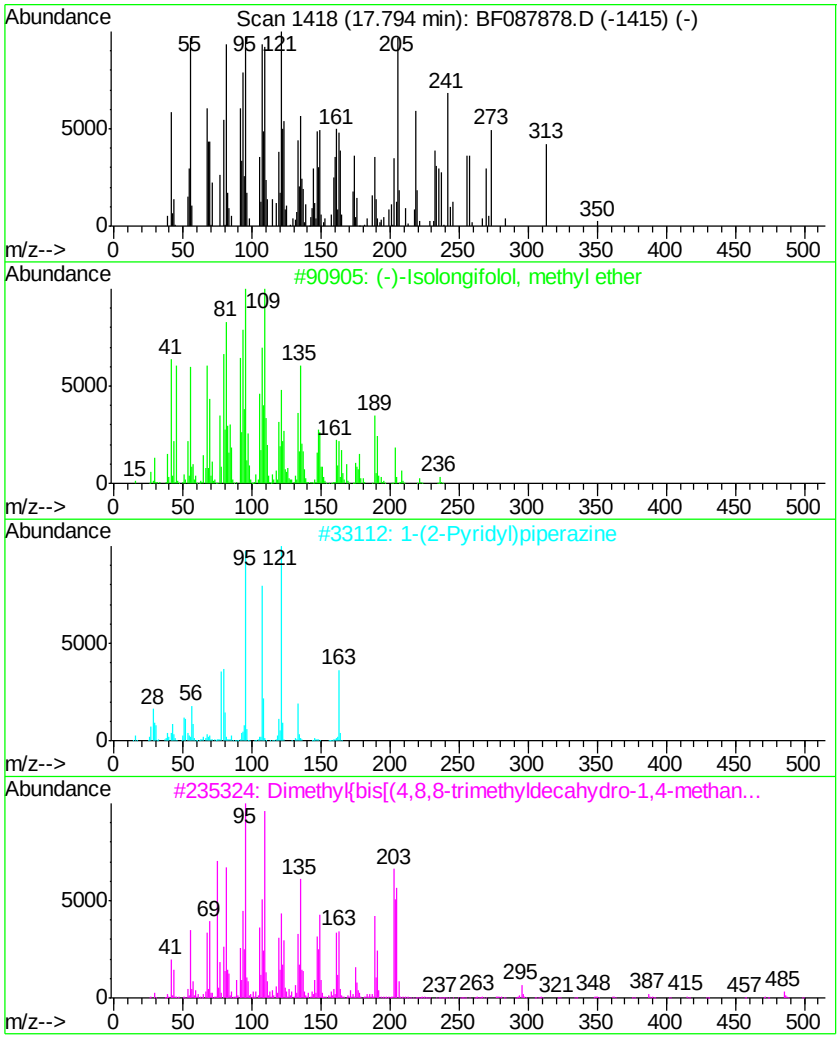
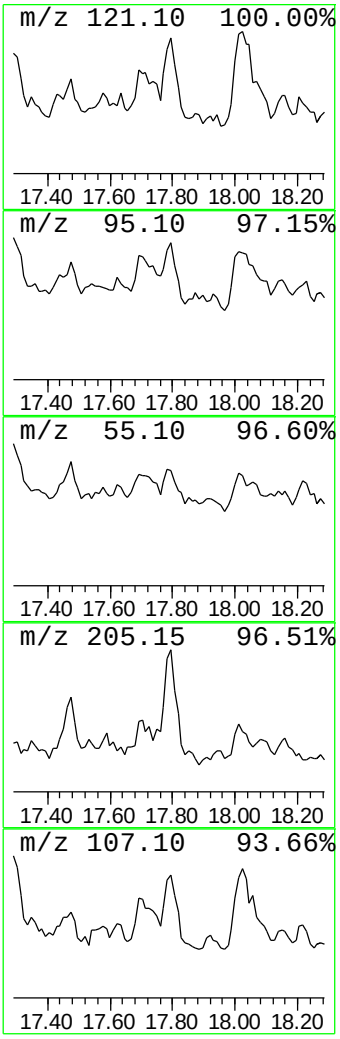
Peak Number 15 unknown17.79 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	4.18 ng	138469	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	38
2	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	30
3	Dimethyl{bis[(4,8,8-trimethyldec...	500	C32H56O2Si	1000364-69-0	27
4	1-Hydroxymethyl-5,8,9-endo-10-ex...	236	C16H28O	1000140-32-9	27
5	1,5-Cyclodecadiene, 1,5-dimethyl...	204	C15H24	015423-57-1	25





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Misc :
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Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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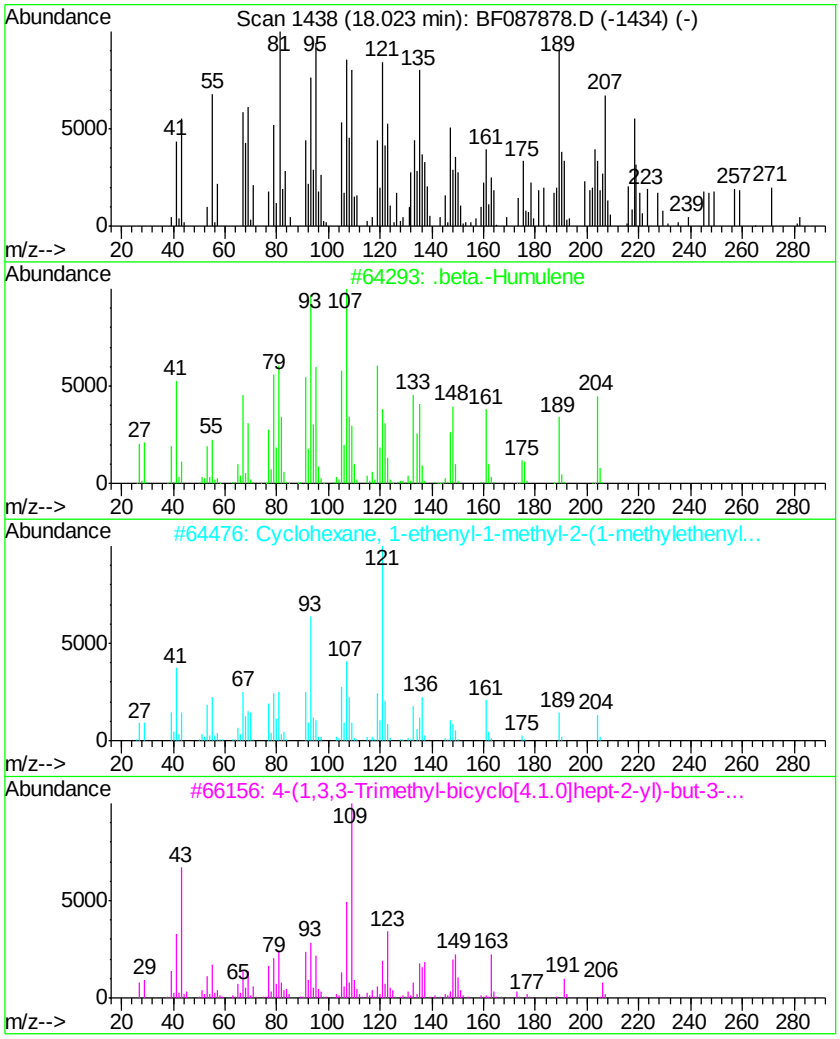
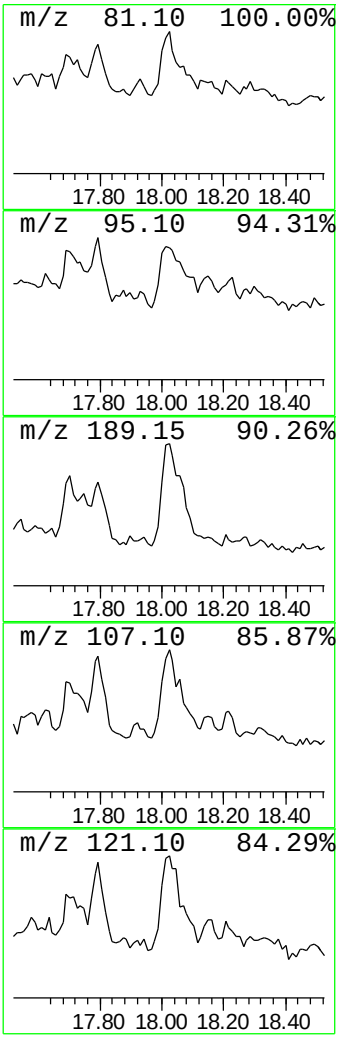
Peak Number 16 .beta.-Humulene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	7.60 ng	251748	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Humulene	204	C15H24	000116-04-1	91
2	Cyclohexane, 1-ethenyl-1-methyl-...	204	C15H24	003242-08-8	46
3	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	45
4	7-Oxabicyclo[4.1.0]heptane, 2,2,...	218	C15H22O	070038-20-9	44
5	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	42





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Sample : H3426-11 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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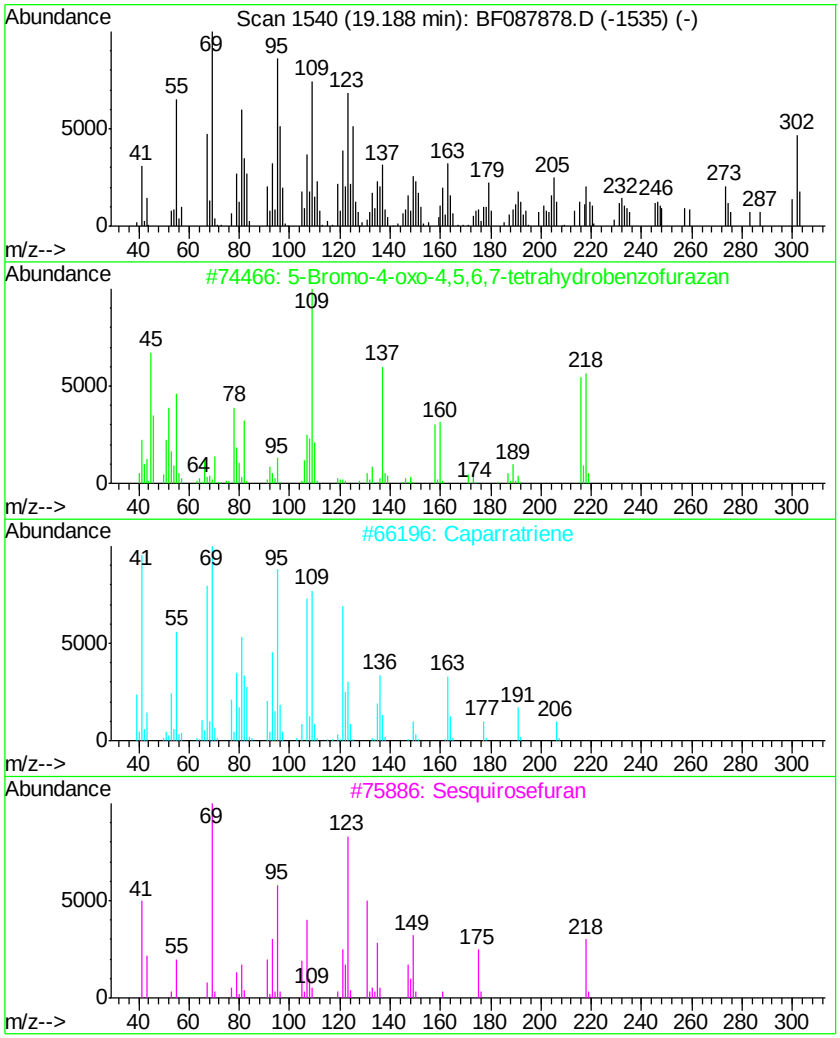
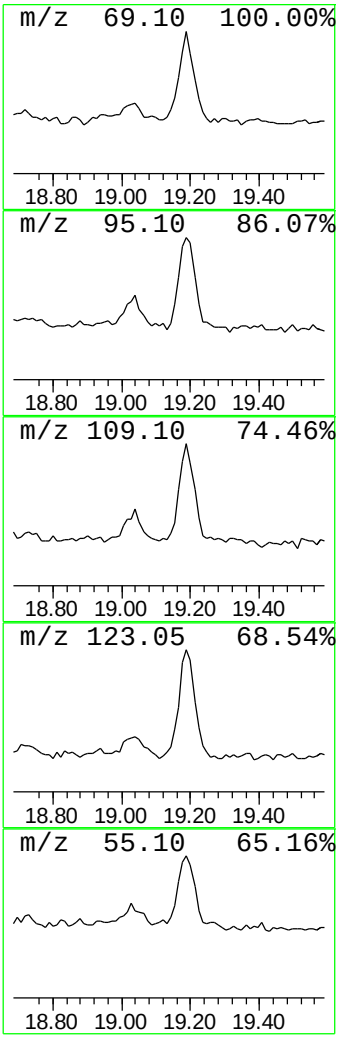
Peak Number 17 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	9.53 ng	315598	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2	Caparratriene	206	C15H26	1000374-08-7	78
3	Sesquirosefuran	218	C15H22O	039007-93-7	38
4	Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	35
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	30





Tentatively Identified Compound (LSC) summary

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Data File : BF087878.D
Acq On : 10 Jun 2016 16:56
Operator : UM/SJ
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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
unknown6.57	6.57	23.6	ng	934069	1	6.97	793330	20.0
E-15-Heptadecenal	14.43	2.4	ng	120083	5	13.95	992201	20.0
Hexadecanamide	14.71	2.2	ng	71936	6	15.36	662125	20.0
Benzo[j]fluoranthene	15.23	3.0	ng	98518	6	15.36	662125	20.0
Heneicosane	15.81	8.9	ng	294244	6	15.36	662125	20.0
16-Hexadecanoyl h...	16.77	3.0	ng	100372	6	15.36	662125	20.0
Dibenzo[def,mno]c...	17.12	2.4	ng	80723	6	15.36	662125	20.0
.beta.-Sitosterol...	17.27	12.1	ng	399665	6	15.36	662125	20.0
unknown17.70	17.70	4.1	ng	135883	6	15.36	662125	20.0
unknown17.79	17.79	4.2	ng	138469	6	15.36	662125	20.0
.beta.-Humulene	18.02	7.6	ng	251748	6	15.36	662125	20.0
5-Bromo-4-oxo-4,5...	19.19	9.5	ng	315598	6	15.36	662125	20.0